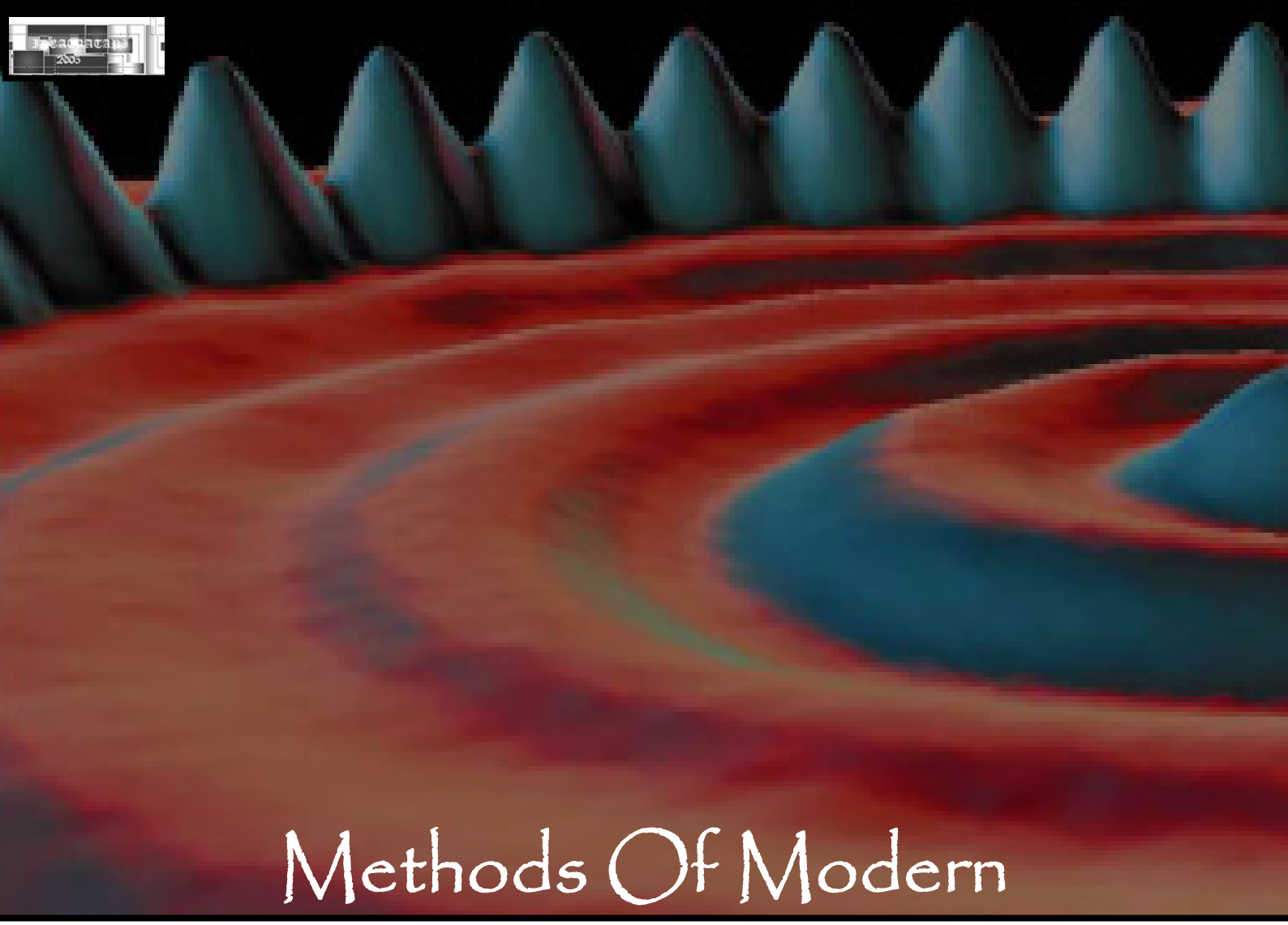
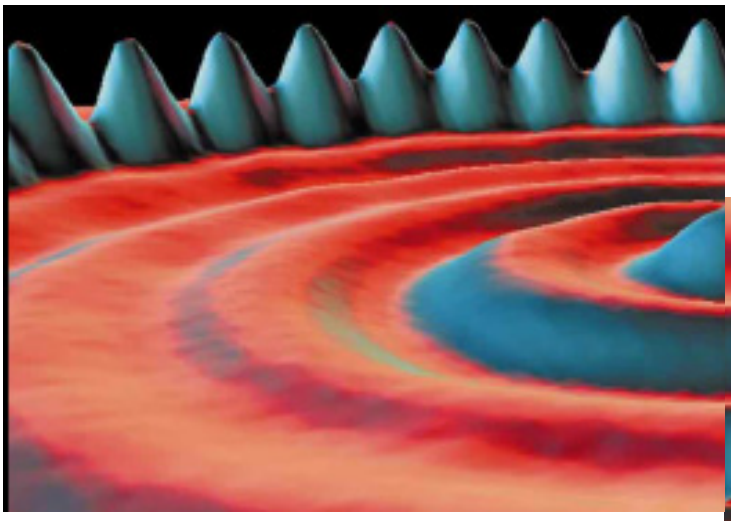


Methods Of Modern Mathematical Physics



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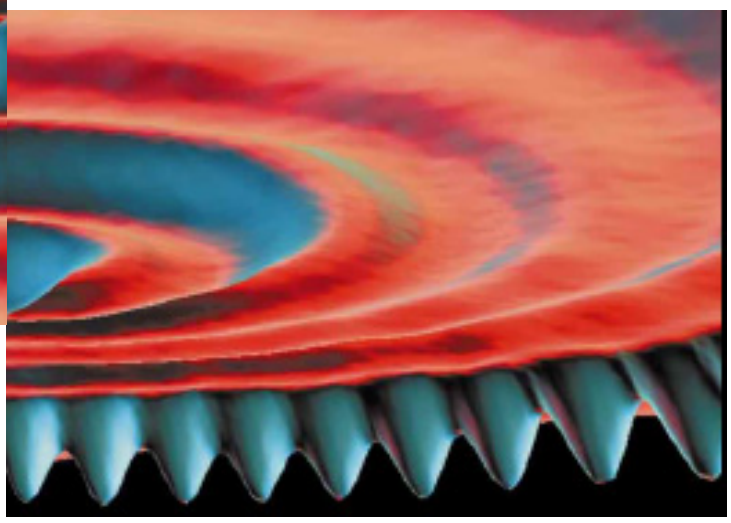

METHODS OF MODERN MATHEMATICAL PHYSICS

I: FUNCTIONAL ANALYSIS

Revised and Enlarged Edition

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To
R. S. Phillips and A. S. Wightman,
Mentors, Colleagues, Friends

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Preface

This book is the first of a multivolume series devoted to an exposition of functional analysis methods in modern mathematical physics. It describes the fundamental principles of functional analysis and is essentially self-contained, although there are occasional references to later volumes. We have included a few applications when we thought that they would provide motivation for the reader. Later volumes describe various advanced topics in functional analysis and give numerous applications in classical physics, modern physics, and partial differential equations.

This revised and enlarged edition differs from the first in two major ways. First, many colleagues have suggested to us that it would be helpful to include some material on the Fourier transform in Volume I so that this important topic can be conveniently included in a standard functional analysis course using this book. Thus, we have included in this edition Sections IX.1, IX.2, and part of IX.3 from Volume II and some additional material, together with relevant notes and problems. Secondly, we have included a variety of supplementary material at the end of the book. Some of these supplementary sections provide proofs of theorems in Chapters II–IV which were omitted in the first edition. While these proofs make Chapters II–IV more self-contained, we still recommend that students with no previous experience with this material consult more elementary texts. Other supplementary sections provide expository material to aid the instructor and the student (for example, "Applications of Compact Operators"). Still other sections introduce and develop new material (for example, "Minimization of Functionals").

It gives us pleasure to thank many individuals:

The students who took our course in 1970–1971 and especially J. E. Taylor for constructive comments about the lectures and lecture notes.

L. Gross, T. Kato, and especially D. Ruelle for reading parts of the manuscript and for making numerous suggestions and corrections.

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MIKE REED
BARRY SIMON

April 1980

Introduction

Mathematics has its roots in numerology, geometry, and physics. Since the time of Newton, the search for mathematical models for physical phenomena has been a source of mathematical problems. In fact, whole branches of mathematics have grown out of attempts to analyze particular physical situations. An example is the development of harmonic analysis from Fourier's work on the heat equation.

Although mathematics and physics have grown apart in this century, physics has continued to stimulate mathematical research. Partially because of this, the influence of physics on mathematics is well understood. However, the contributions of mathematics to physics are not as well understood. It is a common fallacy to suppose that mathematics is important for physics only because it is a useful tool for making computations. Actually, mathematics plays a more subtle role which in the long run is more important. When a successful mathematical model is created for a physical phenomenon, that is, a model which can be used for accurate computations and predictions, the mathematical structure of the model itself provides a new way of thinking about the phenomenon. Put slightly differently, when a model is successful it is natural to think of the physical quantities in terms of the mathematical objects which represent them and to interpret similar or secondary phenomena in terms of the same model. Because of this, an investigation of the internal mathematical structure of the model can alter and enlarge our understanding of the physical phenomenon. Of course, the outstanding example of this is Newtonian mechanics which provided such a clear and coherent picture of celestial motions that it was used to interpret practically all physical phenomena. The model itself became central to an understanding of the physical world and it was difficult to give it up in the late nineteenth century, even in the face of contradictory evidence. A more modern example of this influence of mathematics on physics is the use of group theory to classify elementary particles.

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The analysis of mathematical models for physical phenomena is part of the subject matter of mathematical physics. By analysis is meant both the rigorous derivation of explicit formulas and investigations of the internal mathematical structure of the models. In both cases the mathematical problems which arise lead to more general mathematical questions not associated with any particular model. Although these general questions are sometimes problems in pure mathematics, they are usually classified as mathematical physics since they arise from problems in physics.

Mathematical physics has traditionally been concerned with the mathematics of classical physics: mechanics, fluid dynamics, acoustics, potential theory, and optics. The main mathematical tool for the study of these branches of physics is the theory of ordinary and partial differential equations and related areas like integral equations and the calculus of variations. This classical mathematical physics has long been part of curricula in mathematics and physics departments. However, since 1926 the frontiers of physics have been concentrated increasingly in quantum mechanics and the subjects opened up by the quantum theory: atomic physics, nuclear physics, solid state physics, elementary particle physics. The central mathematical discipline for the study of these branches of physics is functional analysis, though the theories of group representations and several complex variables are also important. Von Neumann began the analysis of the framework of quantum mechanics in the years following 1926, but there were few attempts to study the structure of specific quantum systems (exceptions would be some of the work of Friedrichs and Rellich). This situation changed in the early 1950's when Kato proved the self-adjointness of atomic Hamiltonians and Gårding and Wightman formulated the axioms for quantum field theory. These events demonstrated the usefulness of functional analysis and pointed out the many difficult mathematical questions arising in modern physics. Since then the range and breadth of both the functional analysis techniques used and the subjects discussed in modern mathematical physics have increased enormously. The problems range from the concrete, for example how to compute or estimate the point spectrum of a particular operator, to the general, for example the representation theory of C^*-algebras. The techniques used and the general approach to the subject have become more abstract. Although in some areas the physics is so well understood that the problems are exercises in pure mathematics, there are other areas where neither the physics nor the mathematical models are well understood. These developments have had several serious effects not the least of which is the difficulty of communication between mathematicians and physicists. Physicists are often dismayed at the breadth of background and increasing mathematical sophistication which are required to understand the models. Mathematicians are often frustrated by

their own inability to understand the physics and the inability of physicists to formulate the problems in a way that mathematicians can understand.

A few specific remarks are appropriate. The prerequisite for reading this volume is roughly the mathematical sophistication acquired in a typical undergraduate mathematics education in the United States. Chapter I is intended as a review of background material. We expect that the reader will have some acquaintance with parts of the material covered in Chapters II–IV and have occasionally omitted proofs in these chapters when they seem uninspiring and unimportant for the reader.

The material in this book is sufficient for a two-semester course. Although we taught most of the material in a special one-semester course at Princeton which met five days a week, we do not recommend a repetition of that, either for faculty or students. In order that the material may be easily adapted for lectures, we have written most of the chapters so that the earlier sections contain the basic topics while the later sections contain more specialized and advanced topics and applications. For example, one can give students the basic ideas about unbounded operators in nine or ten lectures from Sections 1–4 of Chapter VIII. On the other hand, by doing the details of the proofs and by adding material from the notes and problems, Chapter VIII could easily become a one-semester course by itself.

Each chapter of this book ends with a long set of problems. Some of the problems fill gaps in the text (these are marked with a dagger). Others develop alternate proofs to the theorems in the text or introduce new material. We have also included harder problems (indicated by a star) in order to challenge the reader. We strongly encourage students to do the problems. It is trite but true that mathematics is learned by doing it, not by watching other people do it.

We hope that these volumes will provide physicists with an access to modern abstract techniques and that mathematicians will benefit by learning the advanced techniques side by side with their applications.

I: Preliminaries

The beginner... should not be discouraged if... he finds that he does not have the prerequisites for reading the prerequisites. *P. Halmos*

I.1 Sets and functions

We assume that the reader is familiar with sets and functions but it is appropriate to standardize our terminology and to introduce here abbreviations that will occur throughout the book.

If X is a set, $x \in X$ means that x is an element of X; $x \notin X$ means that x is not in X. The clause "for all x in X" is abbreviated $(\forall x \in X)$ and "there exists an $x \in X$ such that" is abbreviated $(\exists x \in X)$. The symbol $\{x \mid P(x)\}$ stands for the set of x obeying the condition (or conditions) $P(x)$. If A is a subset of X (denoted $A \subset X$), the symbol $X \backslash A$ represents the complement of A in X, that is $X \backslash A = \{x \in X \mid x \notin A\}$. More generally, if A and B are subsets of X, then $A \backslash B = \{x \mid x \in A, x \notin B\}$. When we discuss sets with a topology, $\bar{A}$ will always denote the closure of the set A. Finally, the set of ordered pairs $\{\langle x, y\rangle \mid x \in X, y \in Y\}$ is called the **Cartesian product** of X and Y and is denoted $X \times Y$.

We will use the words "function" and "mapping" interchangeably. In order to emphasize that certain functions f depend on two variables, we will sometimes write $f(\cdot, \cdot)$. The symbol $f(\cdot, y)$ denotes the function of one variable obtained by picking a fixed value of y for the second variable. A

linear function will also be called an **operator** or a **linear transformation**. Our functions will always be single valued; so a function from a set X to another set Y, denoted by $f: X \to Y$ or $X \xrightarrow{f} Y$ or $x \mapsto f(x)$ will have one and only one value in Y for each $x \in X$. If $A \subset X$, then $f[A] = \{f(x) | x \in A\}$ is a subset of Y and $f^{-1}[B] = \{x | f(x) \in B\}$ is a subset of X if $B \subset Y$. $f[X]$ will usually be called the **range** of f and will be denoted Ran f. X is called the **domain** of f. A function f will be called **injective** (or one-one) if for each $y \in$ Ran f there is at most $x \in X$ such that $f(x) = y$; f is called surjective (or onto) if Ran $f = Y$. If f is both injective and **surjective**, we will say it is **bijective**. The restriction of f to a subset A of its domain will be denoted by $f \restriction A$.

If $X \supset A$ we define the **characteristic function** $\chi_A(x)$ as

$$\chi_A(x) = \begin{cases} 1 & \text{if } x \in A \\ 0 & \text{if } x \notin A \end{cases}$$

There are two set theoretic notions which are slightly deeper than mere notation, so we will discuss them to some extent. A **relation** R on a set X is a subset R of $X \times X$; if $\langle x, y \rangle \in R$, we say that x is related (or R-related) to y and write xRy.

Definition A relation R is called an **equivalence relation** if it satisfies:

(i) $(\forall x \in X)\ xRx$ [reflexive]
(ii) $(\forall x, y \in X)\ xRy$ implies yRx [symmetric]
(iii) $(\forall x, y, z \in X)\ xRy$ and yRz implies xRz [transitive]

The set of elements in X that are related to a given $x \in X$ is called the **equivalence class** of x, denoted usually as $[x]$.

It is easy to prove:

Theorem I.1 Let R be an equivalence relation on a set X. Then each $x \in X$ belongs to a unique equivalence class.

Thus, under an equivalence relation, a set divides up in a natural way into disjoint subsets.

Example 1 (the integers mod 3) Let X be the integers and write xRy if $x - y$ is a multiple of 3. This equivalence relation divides the integers into three equivalence classes:

$$[0] = \{\ldots, -6, -3, 0, 3, 6, \ldots\}$$
$$[1] = \{\ldots, -5, -2, 1, 4, 7, \ldots\}$$
$$[2] = \{\ldots, -4, -1, 2, 5, 8, \ldots\}$$

Example 2 (the real projective line) Let $\mathbb{R}$ denote the real line and let X be the nonzero vectors in $\mathbb{R}^2$ ($= \mathbb{R} \times \mathbb{R}$). We write xRy if there is some $\alpha \in \mathbb{R}$ with $x = \alpha y$. The equivalence classes are lines through the origin (with $\langle 0, 0 \rangle$ removed).

Next, we discuss Zorn's lemma.

Definition A relation on a set X which is reflexive, transitive, and antisymmetric (that is, xRy and yRx implies $x = y$) is called a **partial ordering**. If R is a partial ordering, we often write $x \prec y$ instead of xRy.

Example 3 Let X be the collection of all subsets of a set Y. Define $A \prec B$ if $A \subset B$. Then $\prec$ is a partial ordering.

We use the word "partial" in the above definition because two elements of X need not obey $x \prec y$ or $y \prec x$. If for all x and y in X, either $x \prec y$ or $y \prec x$, X is said to be **linearly ordered**. For example, $\mathbb{R}$ with its usual order $\leq$ is linearly ordered.

Now suppose X is partially ordered by $\prec$ and $Y \subset X$. An element $p \in X$ is called **upper bound** for Y if $y \prec p$ for all $y \in Y$. If $m \in X$ and $m \prec x$ implies $x = m$, we say m is a **maximal element** of X.

Depending on one's starting point, Zorn's lemma is either a basic assumption of set theory or else derived from the basic assumptions (it is equivalent to the *axiom* of choice). We take Zorn's lemma and the rest of set theory as given.

Theorem I.2 (Zorn's lemma) Let X be a nonempty partially ordered set with the property that every linearly ordered subset has an upper bound in X. Then each linearly ordered set has some upper bound that is also a maximal element of X.

Finally, we will use Halmos' ∎ to indicate the conclusion of a proof.

I.2 Metric and normed linear spaces

Throughout this work, we will be dealing with sets of functions or operators or other objects and we will often need a way of measuring the distance

between the objects in the sets. It is reasonable to define a notion of distance that has the most important properties of ordinary distance in $\mathbb{R}^3$.

Definition A **metric space** is a set M and a real-valued function $d(\cdot, \cdot)$ on $M \times M$ which satisfies:

(i) $d(x, y) \geq 0$
(ii) $d(x, y) = 0$ if and only if $x = y$
(iii) $d(x, y) = d(y, x)$
(iv) $d(x, z) \leq d(x, y) + d(y, z)$ [triangle inequality]

The function d is called a **metric** on M.

We often call the elements of a metric space points. Notice that a metric space is a set M together with a metric function d; in general, a given set X can be made into a metric space in different ways by employing different metric functions. When it is not clear from the context which metric we are talking about, we will denote the metric space by $\langle M, d \rangle$, so that the metric is explicitly displayed.

Example 1 Let $M = \mathbb{R}^n$ with the distance between two points $x = \langle x_1, \ldots, x_n \rangle$ and $y = \langle y_1, \ldots, y_n \rangle$ given by

$$d(x, y) = \sqrt{(x_1 - y_1)^2 + \cdots + (x_n - y_n)^2}$$

Example 2 Let M be the unit circle in $\mathbb{R}^2$, that is, the set of all pairs of real numbers $\langle \alpha, \beta \rangle$ with $\alpha^2 + \beta^2 = 1$, and let

$$d_1(\langle \alpha, \beta \rangle, \langle \alpha', \beta' \rangle) = \sqrt{(\alpha - \alpha')^2 + (\beta - \beta')^2}$$

Another possible metric is $d_2[p, p'] =$ arc length between the points p, p' (see Figure I.1).

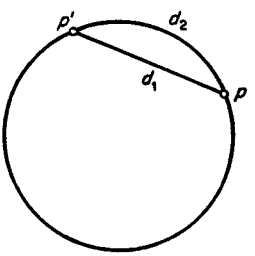

FIGURE I.1 The metrics d_1 and d_2.

Example 3 Let $M = C[0, 1]$, the continuous real-valued functions on $[0, 1]$ with either of the metrics

$$d_1(f, g) = \max_{x \in [0,1]} |f(x) - g(x)| \qquad d_2(f, g) = \int_0^1 |f(x) - g(x)|\, dx$$

Now that we have a notion of distance, we can say what we mean by convergence.

Definition A sequence of elements $\{x_n\}_{n=1}^{\infty}$ of a metric space $\langle M, d\rangle$ is said to **converge** to an element $x \in M$, if $d(x, x_n) \to 0$ as $n \to \infty$. We will often denote this by $x_n \xrightarrow{d} x$ or $\lim_{n\to\infty} x_n = x$. If x_n does not converge to x, we will write $x_n \xrightarrow{d} \!\!\!\!/\;\; x$.

In Example 2, $d_1(p, p') \le d_2(p, p') \le \pi d_1(p, p')$ which we will write $d_1 \le d_2 \le \pi d_1$. Thus $p_n \xrightarrow{d_1} p$ if and only if $p_n \xrightarrow{d_2} p$. But in Example 3, the metrics induce distinct notions of convergence. Since $d_2 \le d_1, f_n \xrightarrow{d_1} f$ implies $f_n \xrightarrow{d_2} f$, but the converse is false. A counterexample is given by the functions g_n defined in Figure I.2, which converge to the zero function in the metric d_2

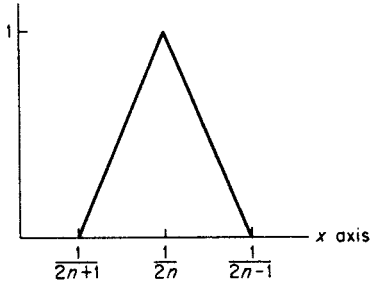

FIGURE I.2 The graph of $g_n(x)$.

but which do not converge in the metric d_1. This may be seen by introducing the important notion of Cauchy sequence.

Definition A sequence of elements $\{x_n\}$ of a metric space $\langle M, d\rangle$ is called a **Cauchy sequence** if $(\forall \varepsilon > 0)(\exists N)$ $n, m \ge N$ implies $d(x_n, x_m) < \varepsilon$.

Proposition Any convergent sequence is Cauchy.

Proof Given $x_n \to x$ and ε, find N so $n \ge N$ implies $d(x_n, x) < \varepsilon/2$. Then $n, m \ge N$ implies $d(x_n, x_m) \le d(x_n, x) + d(x, x_m) < \frac{1}{2}\varepsilon + \frac{1}{2}\varepsilon$. ∎

The reader can prove for himself the following collection of elementary statements:

Theorem I.4 Let $\langle X, d\rangle$ be a metric space:

(a) A set, O, is open if and only if $X\backslash O$ is closed.
(b) $x_m \xrightarrow{d} x$ if and only if for each neighborhood N of x, there exists an M so that $m \geq M$ implies $x_m \in N$.
(c) The set of interior points of a set is open.
(d) The union of a set E with its limit points is a closed set (denoted by $\bar{E}$ and called the **closure** of E).
(e) A set is open if and only if it is a neighborhood of each of its points.

One of the main uses of open sets is to check for convergence using Theorem I.4.b and in particular to check for continuity via the following criteria, the proof of which we leave as an exercise:

Theorem I.5 A function $f(\cdot)$ from a metric space X to another space Y is continuous if and only if for all open sets $O \subset Y$, $f^{-1}[O]$ is open.

Finally, we warn the reader that often in incomplete metric spaces, closed sets may not appear to be closed at first glance. For example, $[\frac{1}{2}, 1)$ is closed in $(0, 1)$ (with the usual metric).

We complete this section with a discussion of two of the central concepts of functional analysis: normed linear spaces and bounded linear transformations.

Definition A **normed linear space** is a vector space, V, over $\mathbb{R}$ (or $\mathbb{C}$) and a function, $\|\cdot\|$ from V to $\mathbb{R}$ which satisfies:

(i) $\|v\| \geq 0$ for all v in V
(ii) $\|v\| = 0$ if and only if $v = 0$
(iii) $\|\alpha v\| = |\alpha|\ \|v\|$ for all v in V and α in $\mathbb{R}$ (or $\mathbb{C}$)
(iv) $\|v + w\| \leq \|v\| + \|w\|$ for all v and w in V

Definition A **bounded linear transformation** (or bounded operator) from a normed linear space $\langle V_1, \|\ \|_1\rangle$ to a normed linear space $\langle V_2, \|\ \|_2\rangle$ is a function, T, from V_1 to V_2 which satisfies:

(i) $T(\alpha v + \beta w) = \alpha T(v) + \beta T(w)$ $(\forall v, w \in V)(\forall \alpha, \beta \in \mathbb{R}$ or $\mathbb{C})$
(ii) For some $C \geq 0$, $\|Tv\|_2 \leq C\|v\|_1$

The smallest such C is called the **norm of** T, written $\|T\|$ or $\|T\|_{1,2}$. Thus

$$\|T\| = \sup_{\|v\|_1 = 1} \|Tv\|_2$$

Since we will study these concepts in detail later, we will not give many examples now but merely note that $\mathbb{R}^n$ with the norm

$$\|\langle x_1, \ldots, x_n \rangle\| = \sqrt{|x_1|^2 + \cdots + |x_n|^2}$$

and $C[0, 1]$ with either the norm

$$\|f\|_\infty = \sup_{x \in [0,1]} |f(x)| \qquad \text{or} \qquad \|f\|_1 = \int_0^1 |f(x)|\, dx$$

are normed linear spaces. Observe also that any normed linear space $\langle V, \|\cdot\| \rangle$ is a metric space when given the distance function $d(v, w) = \|v - w\|$. There is thus a notion of continuity of functions, and for linear functions this is precisely captured by bounded linear transformations. The proof of this fact is left to the reader.

Theorem I.6 Let T be a linear transformation between two normed linear spaces. The following are equivalent:

(a) T is continuous at one point.
(b) T is continuous at all points.
(c) T is bounded.

Definition We say $\langle V, \|\cdot\| \rangle$ is **complete** if it is complete as a metric space in the induced metric.

If $\langle X, \|\cdot\| \rangle$ is a normed linear space, then X has a completion as a metric space by Theorem I.3. Using the fact that X is dense in $\tilde{X}$, it is easy to see that $\tilde{X}$ can be made into a normed linear space in exactly one natural way. All these concepts are well illustrated by the following important theorem and its proof:

Theorem I.7 (the B.L.T. theorem) Suppose T is a bounded linear transformation from a normed linear space $\langle V_1, \|\cdot\|_1 \rangle$ to a complete normed linear space $\langle V_2, \|\cdot\|_2 \rangle$. Then T can be uniquely extended to a bounded linear transformation (with the same bound), $\tilde{T}$, from the completion of V_1 to $\langle V_2, \|\cdot\|_2 \rangle$.

We now return to the functions in Figure I.2. It is easy to see that if $n \neq m$, $d_1(g_n, g_m) = 1$. Thus g_n is not a Cauchy sequence in $\langle C[0, 1], d_1 \rangle$ and therefore not a convergent sequence. Thus, the sequence $\{g_n\}$ converges in $\langle C[0, 1], d_2 \rangle$ but not in $\langle C[0, 1], d_1 \rangle$.

Although every convergent sequence is a Cauchy sequence, the following example shows that the converse need not be true. Let $\mathbb{Q}$ be the rational numbers with the usual metric (that is, $d(x, y) = |x - y|$) and let x^* be any irrational number (that is, $x^* \in \mathbb{R} \backslash \mathbb{Q}$). Find a sequence of rationals x_n with $x_n \to x^*$ in $\mathbb{R}$. Then x_n is a Cauchy sequence of numbers in $\mathbb{Q}$, but it cannot converge in $\mathbb{Q}$ to some $y \in \mathbb{Q}$ (for, if $x_n \to y$ in $\mathbb{Q}$, then $x_n \to y$ in $\mathbb{R}$, so we would have $y = x^*$).

Definition A metric space in which all Cauchy sequences converge is called **complete.**

For example, $\mathbb{R}$ is complete, but $\mathbb{Q}$ is not. It can be shown (Sections I.3 and I.5) that $\langle C[0, 1], d_1 \rangle$ is complete but $\langle C[0, 1], d_2 \rangle$ is not. The example of $\mathbb{Q}$ and $\mathbb{R}$ suggests what we need to do to an incomplete space X to make it complete. We need to enlarge X by adding "all possible limits of Cauchy sequences." The original space X should be dense in the larger space $\tilde{X}$ where:

Definition A set B in a metric space M is called **dense** if every $m \in M$ is a limit of elements in B.

Of course, if the incomplete space is not already contained in a larger complete space (like $\mathbb{Q}$ is contained in $\mathbb{R}$) it is not clear what "all possible limits" means. That this "completion" can be done is the content of a theorem that we shall shortly state; but first some definitions:

Definition A function f from a metric space $\langle X, d \rangle$ to a metric space $\langle Y, \rho \rangle$ is called **continuous at x** if $f(x_n) \xrightarrow{\langle Y, \rho \rangle} f(x)$ whenever $x_n \xrightarrow{\langle X, d \rangle} x$.

We have already had an example of a sequence of elements in $C[0, 1]$ with $f_n \xrightarrow{d_2} 0$ but $f_n \not\xrightarrow{d_1} 0$. Thus the identity function from $\langle C[0, 1], d_2 \rangle$ to $\langle C[0, 1], d_1 \rangle$ is *not* continuous but the identity from $\langle C[0, 1], d_1 \rangle$ to $\langle C[0, 1], d_2 \rangle$ is continuous.

Definition A bijection h from $\langle X, d\rangle$ to $\langle Y, \rho\rangle$ which preserves the metric, that is,

$$\rho(h(x), h(y)) = d(x, y)$$

is called an **isometry**. It is automatically continuous. $\langle X, d\rangle$ and $\langle Y, \rho\rangle$ are said to be **isometric** if such an isometry exists.

Isometric spaces are essentially identical as metric spaces; a theorem concerning only the metric structure of $\langle X, d\rangle$ will hold in all spaces isometric to it.

We now state precisely in which sense an incomplete space can be fattened out to be complete:

Theorem I.3 If $\langle M, d\rangle$ is an incomplete metric space, it is possible to find a complete metric space $\tilde{M}$ so that M is isometric to a dense subset of $\tilde{M}$.

Sketch of proof Consider the Cauchy sequences $\{x_n\}$ of elements of M. Call two sequences, $\{x_n\}$, $\{y_m\}$, equivalent if $\lim_{n\to\infty} d(x_n, y_n) = 0$. Let $\tilde{M}$ be the family of equivalence classes of Cauchy sequences under this equivalence relation. One can show that for any two Cauchy sequences $\lim_{n\to\infty} d(x_n, y_n)$ exists and depends only on the equivalence classes of $\{x_n\}$ and $\{y_n\}$. This limit defines a metric on $\tilde{M}$ and $\tilde{M}$ is complete. Finally, map M into $\tilde{M}$ by taking x into the constant sequence in which each x_n equals x. M is dense in $\tilde{M}$ and the map is isometric. ∎

To complete our discussion of metric spaces, we want to introduce the notions of open and closed sets. The reader should keep the example of open and closed sets on the real line in mind.

Definition Let $\langle X, d\rangle$ be a metric space:

(a) The set $\{x \mid x \in X, d(x, y) < r\}$ is called the **open ball**, $B(y; r)$, of radius r about the point y.

(b) A set $O \subset X$ is called **open** if $(\forall y \in O)(\exists r > 0)\ B(y; r) \subset O$.

(c) A set $N \subset X$ is called a **neighborhood** of $y \in N$ if $B(y; r) \subset N$ for some $r > 0$.

(d) Let $E \subset X$. A point x is called a **limit point** of E, if $(\forall r > 0)$ $B(x; r) \cap (E \backslash \{x\}) \neq \varnothing$, that is, x is a limit point of E if E contains points *other than* x arbitrarily near x.

(e) A set $F \subset X$ is called **closed** if F contains all its limit points.

(f) If $G \subset X$, $x \in G$ is called an **interior point** of G, if G is a neighborhood of x.

Proof Let $\tilde{V}_1$ be the completion of V_1. For each x in $\tilde{V}_1$, there is a sequence of elements $\{x_n\}$ in V_1 with $x_n \to x$ as $n \to \infty$. Since x_n converges, it is Cauchy, so given ε, we can find N so that $n, m > N$ implies $\|x_n - x_m\|_1 \leq \varepsilon / \|T\|$. Then $\|Tx_n - Tx_m\|_2 = \|T(x_n - x_m)\|_2 \leq \|T\| \, \|x_n - x_m\|_1 \leq \varepsilon$ which proves that Tx_n is a Cauchy sequence in V_2. Since V_2 is complete, $Tx_n \to y$ for some y. Set $\tilde{T}x = y$. We must first show that this definition is independent of the sequence $x_n \to x$ chosen. If $x_n \to x$ and $x_n' \to x$, then the sequence $x_1, x_1', x_2, x_2', \ldots \to x$ so $Tx_1, Tx_1', \ldots \to \hat{y}$ for some $\hat{y}$ by the above argument. Thus $\lim Tx_n' = \hat{y} = \lim Tx_n$. Moreover, we can show $\tilde{T}$ so defined is bounded because

$$\begin{aligned} \|\tilde{T}x\|_2 &= \lim_{n \to \infty} \|Tx_n\|_2 && \text{(see Problem 8)} \\ &\leq \overline{\lim_{n \to \infty}} \, C \|x_n\|_1 && \text{(see Appendix to I.2)} \\ &= C\|x\|_1 \end{aligned}$$

Thus $\tilde{T}$ is bounded. The proofs of linearity and uniqueness are left to the reader. ∎

We can use this theorem to give a very elegant definition of the Riemann integral. Let $PC[a, b]$ be the family of bounded piecewise continuous functions on $[a, b]$, which are continuous from the right, that is, $\lim_{x \downarrow y} f(x) = f(y)$ and for which $\lim_{x \uparrow y} f(x)$ exists at each y and is equal to $f(y)$ for all but finitely many y. Norm PC with the norm

$$\|f\|_\infty = \sup_{x \in [a, b]} |f(x)|$$

Let $x_0, \ldots, x_n$ be a partition of the interval $[a, b]$, $x_0 = a$, $x_n = b$. Let $\chi_i(x)$ be the characteristic function of $[x_{i-1}, x_i)$ except for $\chi_n(x)$ which is the characteristic function of $[x_{n-1}, x_n]$. A function on $[a, b]$ of the form $\sum_{i=1}^n s_i \chi_i(x)$ with s_i real is called a **step function** (to see why, draw its graph). The set of all step functions for all possible finite partitions is a normed linear space with the norm

$$\left\| \sum_{i=1}^n s_i \chi_i(x) \right\|_\infty = \sup_{x \in [a, b]} \left| \sum s_i \chi_i(x) \right| = \max_{i = 1, \ldots, n} |s_i|$$

Denote this space by $S[a, b]$. It is a nice exercise (Problem 10) to prove that $S[a, b]$ is dense in $PC[a, b]$. For any step function, $\sum_{i=1}^n s_i \chi_i$, we define

$$I\left(\sum_{i=1}^n s_i \chi_i(x) \right) = \sum_{i=1}^n s_i (x_i - x_{i-1})$$

the intuitive value of the integral $\int [\sum s_i \chi_i(x)] \, dx$. I is a linear transformation from $S[a, b]$ to the real numbers, and because

$$\left| I\left(\sum_{i=1}^{n} s_i \chi_i\right) \right| = \left| \sum s_i (x_i - x_{i-1}) \right|$$

$$\leq \max |s_i| \sum_{i=1}^{n} |x_i - x_{i-1}|$$

$$\leq \|\sum s_i \chi_i\|_\infty (b - a)$$

I is a *bounded* linear transformation. Since the real numbers are complete, I can be uniquely extended to $\tilde{S}$, the completion of S (by the B.L.T. theorem). The extended transformation $\tilde{I}(f)$, restricted to PC is called the Riemann integral and is denoted by

$$I(f) = \int_a^b f\,dx$$

While this method does not appear as the most intuitive definition of the Riemann integral, it will be seen upon reflection that the proof is really just the "usual" proof put into the language of completion and the B.L.T. theorem. It illustrates a main point of general philosophy in functional analysis: In order to define something on a normed linear space, it is often convenient to define it on a dense set and extend it by the B.L.T. theorem. The reader should try his hand at constructing the Riemann–Stieltjes integral (Problem 11). By using the same method, we can define the Riemann integral for continuous functions taking values in any *complete* normed linear space, in particular, for complex-valued functions.

Appendix to 1.2 Lim sup and lim inf

Lim sup and lim inf are notions which may be unfamiliar to the reader, so we summarize their definition and properties.

Definition Let $A \subset \mathbb{R}$ be a nonfinite bounded set. Let lim pt(A) = set of limit points of A. Then the **limit superior of** A is defined by

$$\limsup A \equiv \overline{\lim}\, A = \sup\{x \mid x \in \lim \text{pt}(A)\}$$

Similarly

$$\liminf A \equiv \underline{\lim}(A) = \inf\{x \mid x \in \lim \text{pt}(A)\}$$

Remarks 1. When A is bounded, lim pt(A) is always nonempty by the Bolzano–Weierstrass theorem.

2. If A is not bounded above, one defines $\overline{\lim}\, A = +\infty$. If A is bounded above and lim pt$(A) = \varnothing$ one defines $\overline{\lim}\, A = -\infty$.

3. $\overline{\lim}\, A$ is actually in lim pt(A). For let $b = \overline{\lim}\, A$ and let $\varepsilon > 0$ be given. We can find $a \in$ lim pt(A) so $|b - a| < \varepsilon/2$. Since $a \in$ lim pt(A), we can find $d \in A$ with $|a - d| < \varepsilon/2$; so given ε, we find $d \in A$ with $|b - d| < \varepsilon$, that is, $b \in$ lim pt(A).

$\overline{\lim}\, A$ has a very simple alternative characterization, whose proof we leave to the reader.

Proposition Let $b = \overline{\lim}\, A$. Then for $\varepsilon > 0$, $A \cap \{a \mid a > b + \varepsilon\}$ is finite and $A \cap \{a \mid a > b - \varepsilon\}$ is infinite.

For a sequence $\{a_n\}$, we say $b \in$ lim pt$\{a_n\}$ if for all N and all ε, there is an $n > N$ with $|b - a_n| < \varepsilon$. We define $\overline{\lim}(a_n) = \sup\{b \mid b \in \text{lim pt}\{a_n\}\}$.

Finally, let us summarize the properties of $\overline{\lim}$ (all for bounded sets; it is a useful exercise to decide which extend to unbounded sets).

Proposition

(a) $\overline{\lim}(a_n + b_n) \leq \overline{\lim}\, a_n + \overline{\lim}\, b_n$

(b) $\overline{\lim}\, a_n b_n \leq (\overline{\lim}\, a_n)(\overline{\lim}\, b_n)$ if $a_n, b_n \geq 0$

(c) $\overline{\lim}(ca_n) = c\, \overline{\lim}\, a_n$ if $c > 0$

(d) $\overline{\lim}(ca_n) = c\, \underline{\lim}\, a_n$ if $c < 0$

I.3 The Lebesgue integral

We have just seen that $C[a, b]$ has two quite reasonable metrics on it. In Section I.5 we will see that it is a complete metric space in the metric

$$d_1(f, g) = \sup_{x \in [a, b]} |f(x) - g(x)|$$

In the other metric we considered, $d_2(f, g) = \|f - g\|_1$ with $\|h\|_1 = \int_a^b |h(x)|\, dx$, $C[a, b]$ is *not complete*. To see this for $C[0, 1]$, let f_n be given as in Figure I.3. It is not hard to see that f_n is Cauchy in $\|\cdot\|_1$, but it does not converge to any function in $C[a, b]$; rather, in an *intuitive sense*, it "converges" to the characteristic function of $[\frac{3}{4}, \frac{1}{4}]$ (which is, of course, not in $C[0, 1]$!).

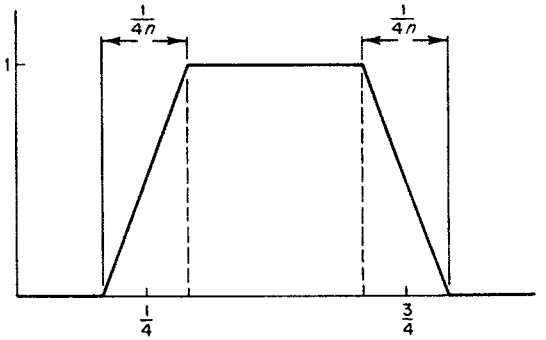

FIGURE I.3 The graph of f_n.

We can always complete $C[a, b]$ in $\|\cdot\|_1$ realizing elements of the completion as equivalence classes of Cauchy sequences of continuous functions; this realization is not noteworthy for its transparency. The example above suggests we might also be able to realize elements of the completion as functions. If we do realize them as functions, we should be able to define the integral $\int_a^b |f(x)|\,dx$ (merely as $d_2(f, 0)$!) for any f in the completion.

The simplest way to realize elements of the completion as functions is to turn the above analysis around: one introduces an extended notion of integral on a bigger space than $C[a, b]$; call it $L^1[a, b]$. We will prove L^1 is complete, so by general arguments the closure of C in L^1 is complete (and it turns out $\bar{C} = L^1$).

Now, how can one extend the notion of Riemann integral? The usual definition of the Riemann integral is based on dividing the *domain* of f into finer and finer pieces. For "nasty" functions, this method does not work and

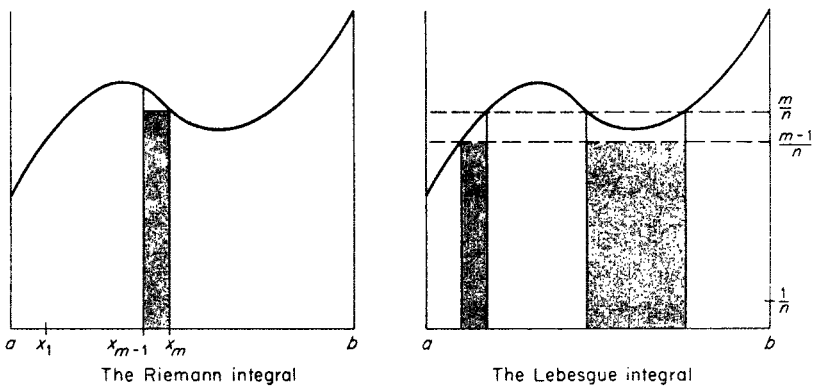

FIGURE I.4

so a different method is needed—the simplest modification is to divide the range into finer and finer pieces (Figure I.4). This method depends more on the function and so has the possibility of working for more types of functions. We are thus interested in sets $f^{-1}[a, b]$ and their size. We suppose we have a size function μ on sets which generalizes $\mu([a, b]) = b - a$. We will shortly return to this size function and see that not all sets have a "size." We will then restrict the types of f by demanding that $f^{-1}[a, b]$ have a "size." Looking at Figure I.4, we define for $f \geq 0$

$$\sum_n(f) = \sum_{m=0}^{\infty} \frac{m}{n} \mu\left(f^{-1}\left[\left[\frac{m}{n}, \frac{m+1}{n}\right)\right]\right)$$

Then $\sum_{2n}(f) \geq \sum_n(f)$ so that $\lim_{n\to\infty} \sum_{2^n}(f) = \sup_n(\sum_{2^n}(f))$ exists (it may be ∞). This limit is defined to be $\int f\,dx$. We remark that for technical purposes (that is, proving theorems!) one makes a different definition which can be shown to agree with this definition only after a lot of work. The definition as $\lim \sum_{2^n}(f)$ is however the best to keep in mind when thinking intuitively.

Thus, we have transferred the problem to one of defining an extended notion of size. We must first decide what sets are to have a size. Why not all sets? There is a classical example (see also Problem 13) which shows that not all sets in $\mathbb{R}^3$ can have a size if we want that size to be invariant under rotations and translations (and not to be trivial, such as assigning zero to all sets): it is possible to break up a unit ball into a finite number of wild pieces, move the pieces around by rotation and translation and reassemble the pieces to get two balls of radius one (Banach–Tarski paradox). Thus, all sets cannot have a size, and so some family $\mathscr{B}$ of sets will be the "measurable sets." What properties do we want $\mathscr{B}$ to have? We would like both $f^{-1}[[0, a)]$ and $f^{-1}[[a, \infty)]$ to be measurable ($f \geq 0$) so we would like $\mathscr{B}$ to have the property: $A \in \mathscr{B}$ implies $\mathbb{R}\backslash A \in \mathscr{B}$. Also, when f is continuous, we want $f^{-1}[(a, b)]$ to be in $\mathscr{B}$, so $\mathscr{B}$ should contain the open sets. Finally, we want to have

$$\mu\left(\bigcup_{n=1}^{\infty} A_n\right) = \sum_{n=1}^{\infty} \mu(A_n)$$

if the A_n are mutually disjoint (to meet our intuitive notion of size) so we would like $\bigcup_{n=1}^{\infty} A_n \in \mathscr{B}$ if each A_n is in $\mathscr{B}$.

Definition The **Borel sets** of $\mathbb{R}$ is the smallest family of subsets of $\mathbb{R}$ with the following properties:

(i) The family is closed under complements.
(ii) The family is closed under countable unions.
(iii) The family contains each open interval.

To see that such a *smallest* family exists we note that if $\{\mathscr{B}_\alpha\}_{\alpha \in A}$ is a collection of families obeying (i), (ii), and (iii), then so does $\bigcap_{\alpha \in A} \mathscr{B}_\alpha$. Thus the intersection of all families obeying (i)–(iii) is the smallest such family.

Now we define the Lebesgue measures of sets in $\mathscr{B}$, the Borel sets in $\mathbb{R}$.

Definition Let $\mathscr{S}$ be the family of all countable unions of disjoint open intervals (which is just the family of open sets) and let

$$\mu\left(\bigcup_{i=1}^{\infty}(a_i, b_i)\right) \equiv \sum_{i=1}^{\infty}(b_i - a_i)$$

(which may be infinite). For any $B \in \mathscr{B}$, define

$$\mu(B) = \inf_{\substack{I \in \mathscr{S} \\ B \subset I}} \mu(I)$$

This notion of size has four crucial properties:

Theorem I.8

(a) $\mu(\varnothing) = 0$

(b) If $\{A_n\}_{n=1}^{\infty} \subset \mathscr{B}$ and the A_n are mutually disjoint ($A_n \cap A_m = \varnothing$, all $m \neq n$), then $\mu\left(\bigcup_{n=1}^{\infty} A_n\right) = \sum_{n=1}^{\infty} \mu(A_n)$.

(c) $\mu(B) = \inf\{\mu(I) \mid B \subset I, I \text{ is open}\}$

(d) $\mu(B) = \sup\{\mu(C) \mid C \subset B, C \text{ is compact}\}$

The infinite sum in (b) contains only positive terms, so it either converges to a finite number or diverges to infinity, in which case we set it equal to ∞. (c) and (d) say that any Borel set can be approximated "from the outside" by open sets and from the inside by compact sets. We remind the reader that *on the real line* a set is compact if and only if it is closed and bounded.

We have thus extended the usual notion of size of intervals and we define the family of functions we will consider in the obvious way:

Definition A function f is called a **Borel function** if and only if $f^{-1}[(a, b)]$ is a Borel set for all a, b.

It is often convenient to allow our functions to take the values $\pm\infty$ on small sets in which case we require $f^{-1}[\{\pm\infty\}]$ to be Borel.

Proposition f is a Borel if and only if, for all $B \in \mathscr{B}$, $f^{-1}[B] \in \mathscr{B}$ (see Problem 14).

This last proposition implies that the composition of two Borel functions is Borel. Many books deal with a slightly larger class of functions than the Borel class. They first define a set M to be measurable if one can write $M \cup A_1 = B \cup A_2$ where B is Borel and $A_i \subset B_i$ with B_i Borel and $\mu(B_i) = 0$ (thus they add and subtract "unimportant" sets from Borel sets). A measurable function is then defined as a function, f, for which $f^{-1}[(a, b)]$ is always measurable. It is no longer true that $f \circ g$ is measurable if f and g are, and many technical problems arise. *In any event, we deal only with Borel sets and functions and use the words Borel and measurable interchangeably.*

Borel functions are closed under many operations:

Proposition (a) If f, g are Borel, then so are $f + g$, fg, $\max\{f, g\}$ and $\min\{f, g\}$. If f is Borel and $\lambda \in \mathbb{R}$, λf is Borel.

(b) If each f_n is Borel, $n = 1, 2, \ldots$, and $f_n(p) \to f(p)$ for all p, then f is Borel.

Since $|f| = \max\{f, -f\}$, $|f|$ is measurable if f is.

As we sketched above, given $f \geq 0$, one can define $\int f\,dx$ (which may be ∞). If $\int |f|\,dx < \infty$, we write $f \in \mathscr{L}^1$ and define $\int f\,dx = \int f_+\,dx - \int f_-\,dx$ where $f_+ = \max\{f, 0\}$; $f_- = \max\{-f, 0\}$. $\mathscr{L}^1(a, b)$ is the set of functions on (a, b) which are in $\mathscr{L}^1$ if we extend them to the whole real line by defining them to be zero outside of (a, b). If $f \in \mathscr{L}^1(a, b)$, we write $\int f\,dx = \int_a^b f\,dx$. We then have:

Theorem I.9 Let f and g be measurable functions. Then

(a) If $f, g \in \mathscr{L}^1(a, b)$, so are $f + g$ and λf, for all $\lambda \in \mathbb{R}$.
(b) If $|g| \leq f$ and $f \in \mathscr{L}^1$, then $g \in \mathscr{L}^1$.
(c) $\int (f + g)\,dx = \int f\,dx + \int g\,dx$ if f and g are in $\mathscr{L}^1$.
(d) $\left|\int f\,dx\right| \leq \int |f|\,dx$ if f is in $\mathscr{L}^1$.
(e) If $f \leq g$, then $\int f\,dx \leq \int g\,dx$, if f and g are in $\mathscr{L}^1$.
(f) If f is bounded and measurable on $-\infty < a < b < \infty$, then $f \in \mathscr{L}^1$ and

$$\left|\int_a^b f\,dx\right| \leq |b - a| \left(\sup_{a \leq x \leq b} |f(x)|\right)$$

This theorem shows that $\int$ has all the nice properties of the Riemann integral even though it is defined for a larger class of functions.

The properties that make the space L^1 (which we will shortly define) complete are the following absolutely essential convergence theorems:

Theorem I.10 (monotone convergence theorem) Let $f_n \geq 0$ be measurable. Suppose $f_n(p) \to f(p)$ for each p and that $f_{n+1}(p) \geq f_n(p)$ all p and n (in which case we write $f_n \nearrow f$). If $\int f_n(p)\, dp < C$ for all n, then $f \in \mathscr{L}^1$ and $\int |f(p) - f_n(p)|\, dp \to 0$ as $n \to \infty$.

Theorem I.11 (dominated convergence theorem) Let $f_n(p) \to f(p)$ for each p and suppose $|f_n(p)| \leq G(p)$ for all n and some $G \in \mathscr{L}^1$. Then $f \in \mathscr{L}^1$ and $\int |f(p) - f_n(p)|\, dp \to 0$ as $n \to \infty$.

In the latter case, we say G dominates the pointwise convergence. That a dominating function exists is crucial. For example, let $f_n(x) = (1/n)\chi_{[-n,n]}(x)$. Then $f_n(x) \to 0$ for each x, but $\int |f_n|\, dx = 2$ so $\int |f_n(x)|\, dx$ does not go to zero. In this case, it is not hard to see that $\sup_n |f_n(x)| = G(x)$ is not in $\mathscr{L}^1$.

We are almost ready to define $\mathscr{L}^1$ as a metric space by letting $\rho(f, g) = \int |f - g|\, dx$. We cannot quite do this because $\int |f - g|\, dx = 0$ does not imply $f \equiv g$ (for example, f and g might differ at a single point). Thus, we first define the notion of almost everywhere (a.e.):

Definition We say a condition $C(x)$ holds almost everywhere (a.e.) if $\{x \mid C(x) \text{ is false}\}$ is a subset of a set of measure zero.

Definition We say two functions $f, g \in \mathscr{L}^1$ are equivalent if $f(x) = g(x)$ a.e. (this is the same as saying $\int |f - g|\, dx = 0$).

Definition The set of equivalence classes in $\mathscr{L}^1$ is denoted by as L^1. L^1 with the norm $\|f\|_1 = \int |f|\, dx$ is a normed linear space.

Thus an element of L^1 is an equivalence class of functions equal a.e. In particular when $f \in L^1$, the symbol $f(x)$ for a particular x does not make sense. Nevertheless we continue to write "$f(x)$" but only in situations where statements are independent of a choice from the equivalence class. Thus, for example, $f_n(x) \to f(x)$ *for almost all* x is independent of the representatives chosen for f and f_n. By this replacement of pointwise convergence with pointwise convergence almost everywhere, the two convergence theorems carry over from $\mathscr{L}^1$ to L^1.

Having cautioned the reader that $f(x)$ is "technically meaningless" for $f \in L^1$, we remark that in *certain special cases* it is meaningful. Suppose $f \in L^1$

has a representative $\tilde{f}$ (that is, $\tilde{f}$ is a function; f an equivalence class of functions) which is continuous. Then no other representative of f is continuous, so it is natural to write $f(x)$ for $\tilde{f}(x)$.

The critical fact about L^1 is:

Theorem I.12 (Riesz–Fisher) L^1 is complete.

Proof Let f_n be Cauchy in L^1. It is enough to prove some subsequence converges (see Problem 3) so pass to a subsequence (also labeled f_n) with $\|f_n - f_{n+1}\|_1 \le 2^{-n}$. Let

$$g_m(x) = \sum_{n=1}^{m} |f_n(x) - f_{n+1}(x)|$$

Let g_∞ be the infinite sum (which may be ∞). Then $g_m \nearrow g_\infty$ and $\int |g_m| \le \sum_{n=1}^{m} \|f_n - f_{n+1}\| \le 1$, so by the monotone convergence theorem, $g_\infty \in L^1$. Thus $|g_\infty(x)| < \infty$ a.e. As a result

$$f_m(x) = f_1(x) - \sum_{n=1}^{m-1} (f_n(x) - f_{n+1}(x))$$

converges pointwise a.e. to a function $f(x)$. Moreover, $|f_m(x)| \le |f_1(x)| + g_\infty(x) \in L^1$ so $f_n \to f$ in L^1 by the dominated convergence theorem. ∎

This proof has a corollary (see Problem 17):

Corollary If $f_n \to f$ in L^1, then some *subsequence* f_{n_i} converges pointwise a.e. to f.

As a final result which brings us full circle to our original motivation:

Proposition $C[a, b]$ is dense (in $\|\cdot\|_1$) in $L^1[a, b]$, i.e. L^1 is the completion of C.

Proof See Problem 18.

We defined $L^1[a, b]$ as a space of real-valued functions. It is often convenient to deal with complex-valued functions, f, whose real and imaginary

parts are in $L^1[a, b]$. When no confusion arises, we will denote this space, with the norm

$$\|f\|_1 = \int_a^b |f| \, dx$$

also by $L^1[a, b]$. The integral of a complex-valued function is defined by

$$\int f \, dx = \int \mathrm{Re}(f) \, dx + i \int \mathrm{Im}(f) \, dx$$

1.4 Abstract measure theory

One of the most important tools which one combines with abstract functional analysis in the study of various concrete models is "general" measure theory, that is, the theory of the last section extended to a more abstract setting.

The simplest way to generalize the Lebesgue integral is to work with functions on the real line and with Borel sets but to generalize the underlying measure; we consider this special case of abstract measure theory first. Recall that the Lebesgue integral was constructed as follows. We started with a notion of size for intervals, $\mu([a, b]) = b - a$, and extended this in a unique way to a notion of size for arbitrary Borel sets. Armed with this notion of size for Borel sets, the integral of Borel functions was obtained by measuring sets of the form $f^{-1}([a, b])$. We found the vector space $L^1([0, 1], dx)$ constructed in the last section is just the completion of $C[0, 1]$ with the metric $d_2(f, g) = \int_0^1 |f(x) - g(x)| \, dx$, where we needed only the Riemann integral to define d_2.

Now suppose an arbitrary monotone function $\alpha(x)$ is given (that is, $x > y$ implies $\alpha(x) \geq \alpha(y)$). It is not hard to see that the limit from the right, $\lim_{\varepsilon \to 0} \alpha(x + |\varepsilon|)$ and the limit from the left, $\lim_{\varepsilon \to 0} \alpha(x - |\varepsilon|)$ exist; we write them as $\alpha(x + 0)$ and $\alpha(x - 0)$ respectively. Since (a, b) does not include the points a and b, it is natural to define $\mu_\alpha((a, b)) = \alpha(b - 0) - \alpha(a + 0)$. From this notion of size for intervals, one can construct a measure μ_α on Borel sets of $\mathbb{R}$, that is, a map $\mu_\alpha : \mathscr{B} \to [0, \infty]$ with $\mu_\alpha(\bigcup B_i) = \sum_{i=1}^{\infty} \mu_\alpha(B_i)$ if $B_i \cap B_j = \varnothing$ and $\mu_\alpha(\varnothing) = 0$. By construction, this measure has the regularity property

$$\begin{aligned} \mu_\alpha(B) &= \sup\{\mu(C) \mid C \subset B, \quad C \text{ compact}\} \\ &= \inf\{\mu(O) \mid B \subset O, \quad O \text{ open}\} \end{aligned}$$

Also, $\mu(C) < \infty$ for any compact set C. A measure with these two regularity properties is called a **Borel measure**. In particular, $\mu_\alpha([a, b]) = \alpha(b + 0) - \alpha(a - 0)$. One can then construct an integral $f \to \int f\, d\mu_\alpha$ (we will also write $\int f\, d\alpha$) which has properties (a)–(e) of Theorem I.9; it is called a Lebesgue–Stieltjes integral. $L^1([a, b], d\alpha)$ and $L^1(\mathbb{R}, d\alpha)$ can be formed as before. These spaces of equivalence classes of functions are complete in the metric $\rho(f, g) = \int |f - g|\, d\alpha$, and analogues of the monotone and dominated convergence theorems hold. The continuous functions $C[a, b]$ form a dense subspace of $L^1([a, b], d\alpha)$; put differently, $L^1([a, b], d\alpha)$ is the completion of $C[a, b]$ with the metric $\rho_\alpha(f, g) = \int_a^b |f - g|\, d\alpha$ where we need only use the Riemann–Stieltjes integral to define ρ_α (see Problem 11).

Let us consider three examples which illustrate the variety of Lebesgue–Stieltjes measures.

Example 1 Suppose α is continuously differentiable. Then $\mu_\alpha(a, b) = \int_a^b (d\alpha/dx)\, dx$ where dx is Lebesgue measure, so it is to be expected (and is indeed true!) that

$$\int f\, d\alpha = \int f\left(\frac{d\alpha}{dx}\right) dx$$

Thus, these measures can essentially be described in terms of Lebesgue measure.

Example 2 Suppose that $\alpha(x)$ is the characteristic function of $[0, \infty)$. Then $\mu_\alpha(a, b) = 1$ if $0 \in (a, b)$ and is 0 if $0 \notin (a, b)$. The measure one gets out is very easy to describe: $\mu_\alpha(B) = 1$ if $0 \in B$, and $\mu_\alpha(B) = 0$ if $0 \notin B$. The reader is invited to construct explicitly the integral and convince himself that

$$\int f\, d\alpha = f(0)$$

This measure $d\alpha$ is known as the Dirac measure (since it is just like a δ function). Let us consider $L^1(\mathbb{R}, d\alpha)$ in this case. In $\mathscr{L}^1$ we have $\rho(f, g) = |f(0) - g(0)|$ so $\rho(f, g) = 0$ if and only if $f(0) = g(0)$. As a result, we see that the equivalence classes in L^1 are completely described by the value $f(0)$ so that $L^1(\mathbb{R}, d\alpha)$ is just a one-dimensional vector space! Notice how different this is from the case of $L^1(\mathbb{R}, dx)$ where the value of a "function" at a single point is not defined (since elements of L^1 are equivalence classes).

Example 3 Our last example makes use of a fairly pathological function, $\alpha(x)$, which we first construct. Let S be the subset of $[0, 1]$

$$S = (\tfrac{1}{3}, \tfrac{2}{3}) \cup (\tfrac{1}{9}, \tfrac{2}{9}) \cup (\tfrac{7}{9}, \tfrac{8}{9}) \cup (\tfrac{1}{27}, \tfrac{2}{27}) \cup \cdots$$



FIGURE I.5 The Cantor set.

that is, remove the middle third of what is not in S at each stage and add it to S, see Figure I.5. The Lebesgue measure of S is $\frac{1}{3} + 2(\frac{1}{9}) + 4(\frac{1}{27}) + \cdots = 1$. Let $C = [0, 1]\backslash S$. It has Lebesgue measure 0. C, which is known as the Cantor set, is easy to describe if we write each $x \in [0, 1]$ in its base three decimal expansion. Then $x \in C$ if and only if this base 3 expansion has no 1's. Thus C is an uncountable set of measure 0. To see this, map C in a one-one way *onto* [0, 1] by changing 2's into 1's and viewing the end result as a base 2 number. Now construct $\alpha(x)$ as follows: set $\alpha(x) = \frac{1}{2}$ on $(\frac{1}{3}, \frac{2}{3})$; $\alpha(x) = \frac{1}{4}$ on $(\frac{1}{9}, \frac{2}{9})$; $\alpha(x) = \frac{3}{4}$ on $(\frac{7}{9}, \frac{8}{9})$, etc.; see Figure I.6. Extend α to [0, 1] by making it con-

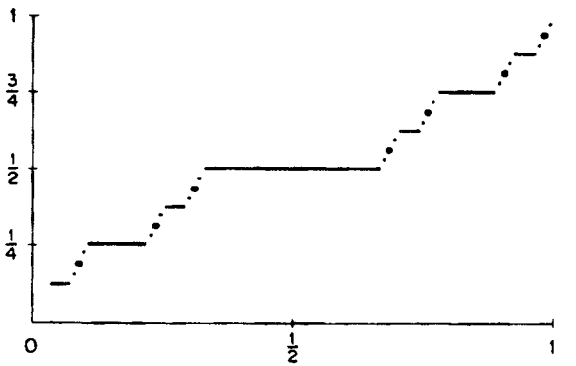

FIGURE I.6 The Cantor function.

tinuous. Then α is a nonconstant continuous function with the strange property that $\alpha'(x)$ exists a.e. (with respect to Lebesgue measure) and is zero a.e. Now, we can form the measure μ_α. Since α is continuous, $\mu_\alpha(\{p\}) = 0$ for any set $\{p\}$ with only one point. Nevertheless, μ_α is concentrated on the set C in the sense that $\mu_\alpha([0, 1]\backslash C) = \mu_\alpha(S) = 0$. On the other hand, the Lebesgue measure of C is zero. Thus μ_α and Lebesgue measure "live" on completely different sets.

In a sense we now make precise, these three examples are models of the most general Lebesgue–Stieltjes measures. Suppose μ is a Borel measure on $\mathbb{R}$.

Definition Let M, N be sets with σ-fields $\mathscr{R}$ and $\mathscr{F}$. A map $T: M \to N$ is called **measurable** (w.r.t. $\mathscr{R}$ and $\mathscr{F}$) if and only if $\forall A \in \mathscr{F}$, $T^{-1}[A] \in \mathscr{R}$. A map $f: M \to \mathbb{R}$ is called measurable if it is measurable w.r.t. $\mathscr{R}$ and the Borel sets of $\mathbb{R}$.

Given a measure μ on a measure space M, we can define $\int f\,d\mu$ for any positive real-valued measurable function on M and we can form $\mathscr{L}^1(M, d\mu)$, the set of integrable functions and $L^1(M, d\mu)$, the equivalence classes of functions in $\mathscr{L}^1$ equal a.e.$[\mu]$. As in the case $\langle M, d\mu\rangle = \langle \mathbb{R}, dx\rangle$, the following crucial theorems hold:

Theorem I.15 (monotone convergence theorem) If $f_n \in \mathscr{L}^1(M, d\mu)$, $0 \le f_1(x) \le f_2(x) \le \cdots$ and $f(x) = \lim_{n\to\infty} f_n(x)$, then $f \in \mathscr{L}^1$ if and only if $\lim_{n\to\infty} \|f_n\|_1 < \infty$ and in that case $\lim_{n\to\infty} \|f - f_n\|_1 = 0$ and $\lim_{n\to\infty} \|f_n\|_1 = \|f\|_1$.

Theorem I.16 (dominated convergence theorem) If $f_n \in L^1(M, d\mu)$, $\lim_{n\to\infty} f_n(x) = f(x)$ a.e.$[\mu]$, and if there is a $G \in L^1$ with $|f_n(x)| \le G(x)$ a.e.$[\mu]$, for all n, then $f \in L^1$ and $\lim_{n\to\infty} \|f - f_n\|_1 = 0$.

Theorem I.17 (Fatou's lemma) If $f_n \in \mathscr{L}^1$, each $f_n(x) \ge 0$ and if $\underline{\lim} \|f_n\|_1 < \infty$, then $f(x) = \underline{\lim} f_n(x)$ is in $\mathscr{L}^1$ and $\|f\|_1 \le \underline{\lim} \|f_n\|_1$.

Note In Fatou's lemma nothing is said about $\lim_{n\to\infty} \|f - f_n\|_1$.

Theorem I.18 (Riesz–Fisher theorem) $L^1(M, d\mu)$ is complete.

One also has the idea of mutually singular:

Definition Let μ, ν be two measures on a space M with σ-field $\mathscr{R}$. We say that μ and ν are mutually singular if there is a set $A \in \mathscr{R}$ with $\mu(A) = 0$, $\nu(M \backslash A) = 0$.

It is useful to take a weaker looking definition of absolute continuity which is essentially the opposite of singular:

Definition We say ν is absolutely continuous w.r.t. μ if and only if $\mu(A) = 0$ implies $\nu(A) = 0$.

That this definition is the same as the previous one is a consequence of:

Theorem I.19 (Radon–Nikodym theorem) ν is absolutely continuous w.r.t. μ if and only if there is a measurable function f so that

$$\nu(A) = \int f(x)\chi_A(x)\, d\mu(x)$$

for any measurable set A. f is uniquely determined a.e. (w.r.t. μ).

Finally the Lebesgue decomposition theorem has an abstract form:

Theorem I.20 (Lebesgue decomposition theorem) Let μ, ν be two measures on a measure space $\langle M, \mathscr{R}\rangle$. Then ν can be written uniquely as $\nu = \nu_{ac} + \nu_{sing}$ where μ and ν_{sing} are mutually singular and ν_{ac} is absolutely continuous w.r.t. μ.

There is one final subject in measure theory which we must consider and that involves changing the order of integration in a multiple integral. We first must consider what functions can be multiply integrated:

Definition Let $\langle M, \mathscr{R}\rangle$, $\langle N, \mathscr{F}\rangle$ be two sets with associated σ-fields. Then the σ-field, $\mathscr{R} \otimes \mathscr{F}$ of subsets of $M \times N$ is defined to be the smallest σ-field containing $\{R \times F \mid R \in \mathscr{R}, F \in \mathscr{F}\}$.

Notice that if $f: M \times N \to \mathbb{R}$ is measurable (w.r.t. $\mathscr{R} \otimes \mathscr{F}$), then for any $m \in M$, the function $n \mapsto f(m, n)$ is measurable (w.r.t. $\mathscr{F}$). If ν is a measure on N such that $\int f(m, n)\, d\nu(n)$ exists for all m, then one can show that $m \mapsto \int f(m, n)\, d\nu(n)$ is measurable (w.r.t. $\mathscr{R}$). There is a direct analogue of the fact that absolute convergent sums can be rearranged at will:

Theorem I.21 (Fubini's theorem) Let f be a measurable function on $M \times N$. Let μ be a measure on M, ν a measure on N. Then

$$\int_M \left(\int_N |f(m, n)|\, d\nu(n) \right) d\mu(m) < \infty$$

if and only if

$$\int_N \left(\int_M |f(m, n)|\, d\mu(m) \right) d\nu(n) < \infty$$

and if one (and thus both) of these integrals is finite, then

$$\int_N \left(\int_M f(m, n)\, d\mu(m) \right) d\nu(n) = \int_M \left(\int_N f(m, n)\, d\nu(n) \right) d\mu(m)$$

First, let $P = \{x \mid \mu(\{x\}) \neq 0\}$, that is, P is the set of **pure points** of μ. Since μ is Borel [$\mu(C) < \infty$ for any compact set], P is a countable set. Define

$$\mu_{pp}(X) = \sum_{x \in P \cap X} \mu(\{x\}) = \mu(P \cap X)$$

Then μ_{pp} is a measure and $\mu_{cont} = \mu - \mu_{pp}$ is positive. μ_{cont} has the property $\mu_{cont}(\{p\}) = 0$ for all p, that is, it has no pure points and μ_{pp} has only pure points in the sense that $\mu_{pp}(X) = \sum_{x \in X} \mu_{pp}(\{x\})$.

Definition A Borel measure μ on $\mathbb{R}$ is called **continuous** if it has no pure points. μ is called a **pure point measure** if $\mu(X) = \sum_{x \in X} \mu(x)$ for any Borel set X.

Thus, we have seen:

Theorem I.13 Any Borel measure can be decomposed uniquely into a sum $\mu = \mu_{pp} + \mu_{cont}$ where μ_{cont} is continuous and μ_{pp} is a pure point measure.

We have thus generalized Example 2 by allowing sums of Dirac measures. Is there any generalization of Examples 1 and 3?

Definition We say that μ is **absolutely continuous with respect to (w.r.t.) Lebesgue measure** if there is a function, f, locally L^1 (that is, $\int_a^b |f(x)|\, dx < \infty$ for any finite interval (a, b)) so that

$$\int g\, d\mu = \int gf\, dx$$

for any Borel function g in $L^1(\mathbb{R}, d\mu)$. We then write $d\mu = f\, dx$.

This definition generalizes Example 1; we will eventually make a different (but equivalent!) definition of absolute continuity.

Definition We say μ is **singular relative to Lebesgue measure** if and only if $\mu(S) = 0$ for some set S where $\mathbb{R} \backslash S$ has Lebesque measure 0.

The fundamental result is:

Theorem I.14 (Lebesgue decomposition theorem) Let μ be a Borel measure. Then $\mu = \mu_{ac} + \mu_{sing}$ in a unique way with μ_{ac} absolutely continuous w.r.t. Lebesgue measure and with μ_{sing} singular relative to Lebesgue measure.

Thus Theorems I.13 and I.14 tell us that any measure μ on $\mathbb{R}$ has a canonical decomposition $\mu = \mu_{pp} + \mu_{ac} + \mu_{sing}$ where μ_{pp} is pure point, μ_{ac} absolutely continuous with respect to Lebesgue measure, and μ_{sing} is *continuous and singular* relative to Lebesgue measure. This decomposition will recur in a quantum-mechanical context where any state will be a sum of bound states, scattering states, and states with no physical interpretation (one of our hardest jobs will be to show that this last type of state does not occur; that is, that certain measures have $\mu_{sing} = 0$; (see Chapter XIII).)

This completes our study of measures on $\mathbb{R}$. The next level of generalization involves measures on sets with some underlying topological structure; we will return to study this case of intermediate generality in Section IV.4. The most general setting lets us deal with an arbitrary set. We first need an abstraction of Borel sets:

Definition A nonempty family $\mathscr{R}$ of subsets of a set M is called a **σ-ring** if and only if

(a) $A_i \in \mathscr{R}$, $i = 1, 2, \ldots$ implies $\bigcup_{i=1}^{\infty} A_i \in \mathscr{R}$.
(b) If $A, B \in \mathscr{R}$, then $A \backslash B \in \mathscr{R}$.

If $M \in \mathscr{R}$, we say that $\mathscr{R}$ is a **σ-field.**

The definition of measure is obvious(!):

Definition A **measure** on a set M with σ-ring $\mathscr{R}$ is a map $\mu: \mathscr{R} \to [0, \infty]$ with the properties:

(a) $\mu(\varnothing) = 0$

(b) $\mu\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} \mu(A_i)$, if $A_i \cap A_j = \varnothing$ for all $i \neq j$.

We shall often speak of the measure space $\langle M, \mu \rangle$ without explicitly mentioning $\mathscr{R}$, but the σ-ring is a crucial element of the definition. Occasionally, we will write $\langle M, \mathscr{R}, \mu \rangle$. For certain pathologically "big" spaces, one wants to use the notion of σ-ring rather than σ-field, but to keep things simple, we will consider measures on σ-fields and will suppose the whole space isn't too big in the sense:

Definition A measure μ on a σ-field $\mathscr{F}$ is called **σ-finite** if and only if $M = \bigcup_{i=1}^{\infty} A_i$ with each $\mu(A_i) < \infty$.

We will suppose all our underlying measures are σ-finite.

In Problem 25, the reader will see that the finiteness of the integral of the absolute value is critical.

Fubini's theorem can be put into perspective by the notion of product measure:

Theorem I.22 Let μ be a σ-finite measure on $\langle M, \mathscr{R} \rangle$ and ν a σ-finite measure on $\langle N, \mathscr{F} \rangle$. Then, there is a unique measure $\mu \otimes \nu$ on $\langle M \times N, \mathscr{R} \otimes \mathscr{F} \rangle$ obeying

$$(\mu \otimes \nu)(R \times F) = \mu(R)\nu(F)$$

(where $0 \cdot \infty = 0$). If f is a measurable function on $M \times N$, then

$$\int_M \left(\int_N |f(m, n)| \, d\nu(n) \right) d\mu(m) < \infty$$

if and only if

$$\int_{M \times N} |f| \, d(\mu \otimes \nu) < \infty$$

and in that case

$$\int_{M \times N} f \, d(\mu \otimes \nu) = \int_M \left(\int_N f \, d\nu \right) d\mu$$

One can describe the measure $\mu \otimes \nu$ quite explicitly. If $M \in \mathscr{R} \times \mathscr{F}$ and $M \subset \bigcup_{i=1}^{\infty} R_i \times F_i$ we have $(\mu \otimes \nu)(M) \leq \sum_{i=1}^{\infty} \mu(R_i)\nu(F_i)$. In fact, for any $M \in \mathscr{R} \times \mathscr{F}$,

$$(\mu \otimes \nu)(M) = \inf \left\{ \sum_{i=1}^{\infty} \mu(R_i)\nu(F_i) \,\middle|\, M \subset \bigcup_{i=1}^{\infty} R_i \times F_i \right\}$$

In particular, we can approximate M with a countable union of rectangles making an arbitrarily small error.

I.5 Two convergence arguments

In this section we single out two "tricks" which we will have occasion to use over and over. While they are elementary and the reader may well have seen them, it seems reasonable to discuss them explicitly.

The first argument, which we will call the $\varepsilon/3$ argument, is best seen in the proof of:

Theorem I.23 Let $C[a, b]$ be the continuous functions on $[a, b]$ with the metric

$$d_1(f, g) = \sup_{a \le x \le b} |f(x) - g(x)|$$

induced by the norm $\|f\|_\infty = d_1(f, 0)$. Then $C[a, b]$ with the norm $\|\cdot\|_\infty$ is complete.

Proof Let f_n be a $\|\cdot\|_\infty$-Cauchy sequence. Then, for any fixed $x \in [a, b]$, $|f_n(x) - f_m(x)| \le \|f_n - f_m\|_\infty \to 0$ as $n, m \to \infty$ so $f_n(x)$ is a Cauchy sequence of real numbers. Since the reals are complete, for each x there is a number, $f(x)$, with $f_n(x) \to f(x)$. Given ε, find N so $n, m \ge N$ implies $\|f_n - f_m\|_\infty \le \varepsilon$. Then

$$\begin{aligned} \sup_{a \le x \le b} |f(x) - f_N(x)| &= \sup_{a \le x \le b} \lim_{n \to \infty} |f_n(x) - f_N(x)| \\ &\le \sup_{a \le x \le b} \sup_{n \ge N} |f_n(x) - f_N(x)| \\ &= \sup_{n \ge N} \|f_n - f_N\|_\infty \le \varepsilon \end{aligned}$$

Thus, if we can show that $f \in C[a, b]$, we can conclude that $\|f - f_n\|_\infty \to 0$ so $f_n \to f$ in $C[a, b]$.

We are thus left with proving that f is continuous, or put differently that "a uniform limit of continuous functions is continuous." Fix $x \in [a, b]$ and $\varepsilon > 0$. We want to find δ so $|x - y| < \delta$ implies $|f(x) - f(y)| < \varepsilon$. Pick n so that $\|f_n - f\|_\infty < \varepsilon/3$. Now, since f_n is continuous, pick δ so that $|x - y| < \delta$ implies $|f_n(x) - f_n(y)| < \varepsilon/3$. Then $|x - y| < \delta$ implies

$$\begin{aligned} |f(x) - f(y)| &\le |f(x) - f_n(x)| + |f_n(x) - f_n(y)| + |f_n(y) - f(y)| \\ &< \tfrac{1}{3}\varepsilon + \tfrac{1}{3}\varepsilon + \tfrac{1}{3}\varepsilon \end{aligned}$$

Thus f is continuous. ∎

What is the essence of the $\varepsilon/3$ argument? We had a family of convergent sequences $f_n(x) \to f(x)$ for each x and had *uniform control on the rate of convergence*, that is, control independent of the object x that parametrized the family. We also had some information on the behavior of $f_n(x)$ for fixed n as the parameter x varied *but this information was not necessarily uniform in n.* What we did is pictorially indicated in Figure I.7; one could also call the $\varepsilon/3$ argument the "up, over, and around" proof. In the next section we will consider what happens when one has no uniform information on the rate of convergence but instead has uniform control on how $f_n(x)$ behaves as x varies (uniform in n). There we will see an $\varepsilon/3$ argument also works. For further examples of the $\varepsilon/3$ trick, see Problems 27, 29.

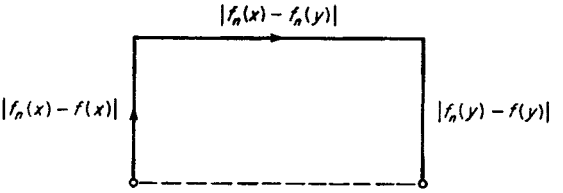

FIGURE I.7 The $\varepsilon/3$ argument.

The second argument which we refer to as the "diagonal sequence trick" is illustrated in:

Theorem I.24 Let $f_n(m)$ be a sequence of functions on the positive integers which is uniformly bounded, i.e. $|f_n(m)| \leq C$ for all n, m. Then there is a subsequence $\{f_{\hat{n}(i)}(m)\}_{i=1}^{\infty}$ so that for each fixed m, $f_{\hat{n}(i)}(m)$ converges as $i \to \infty$.

Proof Consider the sequence $f_n(1)$. It is a bounded set of numbers, so we can find a subsequence $f_{n_1(i)}$ so $f_{n_1(i)}(1) \to f_\infty(1)$, for some number $f_\infty(1)$. Now consider the sequence $f_{n_1(i)}(2)$. We can find a subsequence $f_{n_2(i)}(2) \to f_\infty(2)$ as $i \to \infty$. Proceeding inductively, we find successive subsequences, $f_{n_k(i)}$ so that (a) $f_{n_{k+1}(i)}$ is a subsequence of $f_{n_k(i)}$ and (b) $f_{n_k(i)}(k) \to f_\infty(k)$ as $i \to \infty$. Thus, in particular, $f_{n_k(i)}(j) \to f_\infty(j)$ as $i \to \infty$ for $j = 1, 2, \ldots, k$. To get a subsequence $f_{\hat{n}(i)}$ converging for each j, one is tempted to try to take the limit of the horizontal sequence (see Figure I.8a) but that won't work! (for it may happen $n_k(1) \to \infty$). The simple way out is to take the diagonal sequence $\hat{n}(k) = n_k(k)$. Then $f_{\hat{n}(k)}, f_{\hat{n}(k+1)}, \ldots$ is a subsequence of $f_{n_k(i)}$ so $f_{\hat{n}(i)}(k) \to f_\infty(k)$ as $i \to \infty$ for any k. ∎

I.6 Equicontinuity

We have just seen that one can control the x dependence of $\lim_{n\to\infty} f_n(x)$ if one is given information on the approach to the limit which is uniform in x. In this section we study what happens when the given information is instead uniform in n; what we will see is that one can obtain not only information about the x behavior of the limit but that one can also turn weak information about the approach to the limit into stronger information. We first isolate the notion of "control on the x behavior uniform in n."

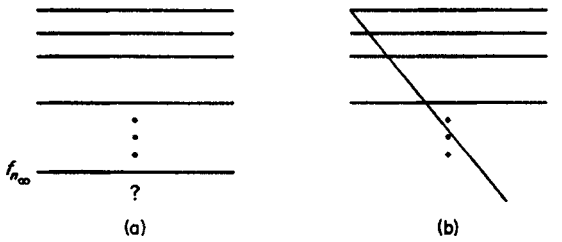

FIGURE I.8 The diagonal trick.

Definition Let $\mathscr{F}$ be a family of functions from a metric space $\langle X, \rho\rangle$ to another metric space $\langle Y, d\rangle$. We say $\mathscr{F}$ is an **equicontinuous family** if and only if

$$(\forall\varepsilon)(\forall x \in X)(\exists\delta)(\forall f \in \mathscr{F})\ \rho(x, x') < \delta \quad \text{implies} \quad d(f(x), f(x')) < \varepsilon.$$

We say $\mathscr{F}$ is a **uniformly equicontinuous family** if and only if

$$(\forall\varepsilon)(\exists\delta)(\forall x \in X)(\forall f \in \mathscr{F})\ \rho(x, x') < \delta \quad \text{implies} \quad d(f(x), f(x')) < \varepsilon.$$

For comparison sake, note that to say all $f \in \mathscr{F}$ are continuous means $(\forall\varepsilon)(\forall x \in X)(\forall f \in \mathscr{F})(\exists\delta)\rho(x, x') < \delta$ implies $d(f(x), f(x')) < \varepsilon$. Thus, for mere continuity, δ can depend on f and x (as well as ε), while equicontinuity says δ is independent of f; finally uniform equicontinuity says δ is dependent only on ε.

As promised, it is easy to turn information about $f_n(x)$, uniform in n into information about the limit:

Theorem I.25 Let f_n be a sequence of functions from one metric space to another with the property that the family $\{f_n\}$ is equicontinuous. Suppose that $f_n(x) \to f(x)$ pointwise for each x. Then f is continuous.

Proof Given ε and x, choose δ so $\rho(x, x') < \delta$ implies $d(f_n(x), f_n(x')) < \frac{1}{2}\varepsilon$ for all n. Since d is continuous, we have $d(f(x), f(x')) = \lim_{n\to\infty} d(f_n(x), f_n(x'))$ so $\rho(x, x') < \delta$ implies $d(f(x), f(x')) \le \varepsilon/2 < \varepsilon$. ∎

The proof makes it clear that if $\{f_{n,m}\}$ is an equicontinuous family and for each m, $\lim_{n\to\infty} f_{n,m} \equiv f_m$ exists, then $\{f_m\}$ is an equicontinuous family. Equicontinuity has a crucial consequence which we will see combines nicely with the diagonal sequence trick:

Theorem I.26 Let $\{f_n\}$ be an equicontinuous family of functions from one metric space $\langle X, \rho\rangle$ to another $\langle Y, d\rangle$ with Y complete. Suppose that for

a dense set $D \subset X$, we know $f_n(x)$ converges for all $x \in D$. Then $f_n(x)$ converges for all $x \in X$. (Note that by Theorem I.25, the limit function is continuous.)

Proof See Problem 29.

Theorem I.26 tells us that, in general, pointwise convergence on a dense set combined with equicontinuity implies pointwise convergence everywhere. More spectacularly, for a sequence of functions on [0, 1] (see Problem 30), uniform equicontinuity and pointwise convergence imply *uniform convergence*:

Theorem I.27 Let $\{f_n\}$ be a uniformly equicontinuous family of functions on [0, 1]. Suppose that $f_n(x) \to f(x)$ for each x in [0, 1]. Then $f_n(x) \to f(x)$ uniformly in x.

Proof Let ε be given. Choose δ so that $|x - y| < \delta$ implies $|f_n(x) - f_n(y)| < \varepsilon/3$ for all n. Now choose $y_1, \ldots, y_m$ so that every point of [0, 1] is within δ of some y_i. Since $y_1, \ldots, y_m$ is a finite set, we can find n so $n > N$ implies $|f_n(y_i) - f(y_i)| < \varepsilon/3$; $i = 1, \ldots, m$. By an $\varepsilon/3$ argument, $\|f_n - f\|_\infty < \varepsilon$ for all $n > N$. ∎

For functions on [0, 1], every equicontinuous family is uniformly equicontinuous (Problem 31).

We can combine the convergence theorems (Theorems I.26 and I.27), the diagonalization trick of Section I.5 and the above remark (Problem 31) to prove the beautiful:

Theorem I.28 (Ascoli's theorem) Let f_n be a family of uniformly bounded equicontinuous functions on [0, 1]. Then some subsequence $f_{n(i)}$ converges uniformly on [0, 1].

Proof Let $q_1, q_2, \ldots$ be a numbering of the rationals. Since the f_n's are uniformly bounded, $|f_n(q_m)| \leq C$ for all m and n. Thus, by the diagonalization trick, we can find a subsequence with $f_{n(i)}(q_m)$ converging as $i \to \infty$ for each m. By Theorem I.26, the $f_{n(i)}$ converge pointwise everywhere and then by Theorem I.27, they are uniformly convergent. ∎

At this point, we discuss no applications in detail. However, we mention two examples to which we shall return which show the variety of applications: In Section V.1, we define a metric on all functions, $\mathcal{O}_D$, analytic in a region D. In Theorem V.25 we use equicontinuity arguments to prove that certain

subsets of $\mathcal{O}_D$ are compact. In Chapter XX, we will discuss the limit of the free energy per unit volume of a "lattice gas" in a box as the volume goes to infinity. Our proof that this limit exists for a large class of interactions will proceed in three steps: (1) The interactions will be given a metric and it will be shown that strictly finite range interactions are dense in all "allowable" interactions in this metric. (2) If for fixed volume Λ the free energy per unit volume F_Λ is treated as a function on the metric space of allowable interactions, the $\{F_\Lambda\}$ are equicontinuous. (3) The $\lim_{\Lambda\to\infty} F_\Lambda(\Phi)$ will be shown to exist if Φ is a finite range interaction. Then equicontinuity arguments will be used to tell us that $\lim_{\Lambda\to\infty} F_\Lambda(\Phi)$ exists for any allowable interaction Φ (and the limit will be continuous in Φ).

NOTES

Section I.1 For a discussion of the subtleties of Zorn's lemma, the axiom of choice, etc. intended for the novice, we recommend: P. R. Halmos, *Naive Set Theory*, Van Nostrand–Reinhold, Princeton, New Jersey, 1960.

Section I.2 For additional discussion of metric space notions, see A. Gleason, *Introduction to Abstract Analysis*, Addison-Wesley, Reading, Massachusetts, 1966, or A. Kolmogorov and S. Fomin, *Elements of the Theory of Functional Analysis*, Vol. I, Graylock Press, 1957. For normed linear spaces (and in particular for our discussion of the Riemann integral) see J. Dieudonné, *Foundations of Modern Analysis*, Academic Press, New York and London, 1960 or L. Loomis and S. Sternberg, *Advanced Calculus*, Addison–Wesley, Reading, Massachusetts, 1968.

Sections I.3, I.4 For a discussion of Lebesgue Integration, see J. Williamson, *Introduction to the Lebesgue Integral*, Holt, New York, 1962 or W. Rudin, *Principles of Modern Analysis*, McGraw-Hill, New York, 1963. For abstract measure theory we particularly recommend S. K. Berberian, *Measure and Integration*, Macmillan, New York, 1965 and H. Royden, *Real Analysis*, Macmillan, New York, 1968. See also P. Halmos: *Measure Theory*, Van Nostrand, Reinhold, Princeton, New Jersey, 1950; N. Dunford and J. Schwartz, *Linear Operators*, Chapter 3, Wiley (Interscience), New York, 1958.

For a discussion of the Banach–Tarski paradox, see R. Rosenblum, *Elements of Mathematical Logic*, p. 150, Dover, New York, 1950, or R. Robinson, *Fund. Math.*, 34 (1947), 246.

We note that one can construct all Borel sets as follows: Start with the open sets and their complements, the closed sets. Add countable unions of closed sets, called F_σ sets and their complements (countable intersections of open sets) called G_δ sets. Then add countable unions of G_δ's called $G_{\delta\sigma}$'s and their complements $F_{\sigma\delta}$'s. Next add $G_{\delta\sigma\delta}$, etc. *After countably many steps one is still not done*, for a union of one G_δ, one $F_{\sigma\delta}$, one $G_{\delta\sigma\delta}$, ... may not have been included. In the end transfinite induction up to the first uncountable ordinal is needed.

As the problems show, the Borel functions are the smallest family closed under pointwise

limits and containing all continuous functions. As with the Borel sets, their construction requires transfinite induction. We note however that, given any Borel measure μ, any Borel function f is equal almost everywhere (w.r.t. μ) to a pointwise limit of continuous functions (Problems 18 and 19).

By removing the middle 2^n-ths at the nth step in [0, 1], one can construct a closed set of positive measure with an empty interior.

The approach to measures on topological spaces (rather than abstract spaces) which we discuss in Section IV.4, is fashionable with the French School. See N. Bourbaki, *Intégration*, Chapters 1–8, Hermann, Paris, (1952, 1956, 1959, 1963) or (for a beautiful and brief discussion) L. Nachbin, *The Haar Integral*, Chapter I, Van Nostrand–Reinhold, Princeton, New Jersey, 1965.

Section I.6 The natural setting for Ascoli's theorem is functions on an arbitrary compact metric space, or more generally, a second countable compact uniform space (which is actually always metrizable), for example, a compact topological group.

The idea of using equicontinuity in establishing the existence of the thermodynamic limit goes back at least as far as R. B. Griffiths: "A Proof that the Free Energy of a Spin System Is Extensive," *J. Math. Phys.* **5** (1964), 1215–1222. The proof we outlined for lattice gases, which we discuss in Chapter XX, is due to G. Gallavotti and S. Miracle: "Statistical Mechanics of Lattice Systems," *Commun. Math. Phys.* **5** (1967), 317–324.

In analytic function theory, equicontinuity is really behind one of the proofs of the Riemann mapping theorem, see e.g. L. Ahlfors, *Complex Analysis*, pp. 172–174, McGraw-Hill, New York, 1953, where sets of equicontinuous functions are called "normal families."

PROBLEMS

1. Find a counterexample to the statement: Every symmetric, transitive relation is reflexive. What is wrong with the proof "xRy and yRx implies xRx (by transitivity)"?

†*2.* Verify that the proposed metrics of Examples 1–3 in Section 1.2 are in fact metrics.

3. Let x_n be a Cauchy sequence in a metric space $\langle X, \rho\rangle$. Suppose that for some subsequence $x_{n(l)}$, $x_{n(l)} \xrightarrow{l\to\infty} x_\infty$. Prove that $x_n \to x_\infty$.

4. Let x_n be a sequence in a metric space and let x_∞ be given. Suppose that every subsequence of x_n has a sub-subsequence converging to x_∞. Prove that $x_n \to x_\infty$.

†*5.* Fill in the details of the proof of Theorem I.3.

†*6.* Prove Theorems I.4 and I.5.

†*7.* Prove Theorem I.6.

8. Prove: If $x_n \to x_\infty$ in a metric space $\langle X, d\rangle$, then for any x, $\lim_{n\to\infty} d(x, x_n) = d(x, x_\infty)$.

†*9.* Complete the proof of Theorem I.7.

†*10.* Prove $S[a, b]$ is dense in $PC[a, b]$ in the $\|\cdot\|_\infty$ norm.

11. (a) Let α be a function on $[0, 1]$. α is said to be of **bounded variation** if there is a C so that

$$\sum_{i=1}^{n-1} |\alpha(x_{i+1}) - \alpha(x_i)| \leq C$$

for any sequence $0 \leq x_1 \leq x_2 \leq \cdots \leq x_n \leq 1$. Prove that any monotone function is of bounded variation.

(b) Define I_α on $S[0, 1]$ by

$$I_\alpha\left(\sum_{i=1}^{n} s_i \chi_i\right) = \sum_{i=1}^{n} s_i[\alpha(x_i) - \alpha(x_{i-1})]$$

Prove I_α is a B.L.T. if and only if α is of bounded variation.

(c) Let α be of bounded variation on $[0, 1]$. Construct a Riemann–Stieltjes integral $\int f \, d\alpha$.

†*12.* Prove the various properties of $\overline{\lim}$ and $\underline{\lim}$ given in the appendix to Section I.2.

13. Construct a set V (the Vitali set) as follows: Call two numbers $x, y \in [0, 1)$ equivalent if $x - y$ is rational. Let V consist of exactly one number from each equivalence class. Let μ be Lebesgue measure. Prove V is not Lebesgue measurable. (Hint: Prove $[0, 1)$ is a disjoint union of "translates" of V.)

†*14.* (a) Let f be a Borel function Prove $f^{-1}[B] \in \mathscr{B}$ for any $B \in \mathscr{B}$.

(b) Let f and g be Borel functions. Prove that $f \circ g$ is Borel.

15. (a) Let $\lim_{n\to\infty} r_n = r$ for r_n, r real numbers. Prove that

$$r = \sup_m (\inf_{n>m} r_n)$$

(b) Prove that if f_n is a sequence of functions and $f(x) = \inf f_n(x)$, then

$$f^{-1}[[a, \infty)] = \bigcap_{n=1}^{\infty} f_n^{-1}[[a, \infty)] \qquad f^{-1}[(a, \infty)] = \bigcup_{m=1}^{\infty} f^{-1}[[a + 1/m, \infty)]$$

Conclude that the infimum of any sequence of Borel functions is Borel.

(c) Using (a) and (b), prove that any pointwise limit of a sequence of Borel functions is a Borel function.

(d) Using (a), prove the dominated convergence theorem from the monotone convergence theorem.

**16.* Prove that the bounded Borel functions on $[0, 1]$ are the smallest family $\mathscr{F}$ which includes $C[0, 1]$ and has the property: If f_n is a *sequence* of uniformly bounded functions in $\mathscr{F}$ and $f_n \to f$ pointwise, then $f \in \mathscr{F}$.

†*17.* Prove the corollary to Theorem I.12.

†*18.* (a) Prove that for any open set A in $[0, 1]$, χ_A is an L^1 limit of continuous functions.

(b) Let B be a Borel set in $[0, 1]$. Prove χ_B is an L^1 limit of functions χ_A with A open (use the regularity of Lebesgue measure).

(c) Prove $C[a, b]$ is L^1 dense in $L^1[a, b]$.

*19. (a) Let $f_n \to f$ pointwise with f_n continuous. Prove $f^{-1}[(a, \infty)]$ is a F_σ set (that is, a union of closed sets). (Hint: Use Problem 15a.)
(b) Prove that every Borel set on the real line is equal a.e. (w.r.t. Lebesgue measure) to an F_σ set and also equal a.e. to a G_δ set.

*20. A function f is called a jump function if it is monotone and continuous except at a countable number of points (jumps) and if f is piecewise constant on the complement of these jumps. f is called singular if f' exists a.e. and is zero a.e. f is called absolutely continuous if, given ε, we can find δ so that for any n

$$\sum_{i=0}^{n} |x_{2i+1} - x_{2i}| < \delta$$

for points $x_0 < x_1 < \ldots < x_{2n+1}$ implies

$$\sum_{i=0}^{n} |f(x_{2i+1}) - f(x_{2i})| < \varepsilon$$

Prove that any monotone function α on $[0, 1]$ can be written (uniquely) $\alpha = \alpha_{pp} + \alpha_{sing} + \alpha_{ac}$ where α_{pp} is a jump function, α_{sing} is singular and continuous, and α_{ac} is absolutely continuous.

21. Let α be a monotone function. Suppose $\alpha'(x)$ exists a.e. Prove $\alpha(b) - \alpha(a) \geq \int_a^b \alpha'(x)\, dx$. Does equality always hold?

†22. Prove that σ-rings are closed under countable intersections.

23. (a) Let $\mathscr{S}$ be a family of substs of M. Prove there is a smallest σ-field $\mathscr{F}$ with $\mathscr{S} \subset \mathscr{F}$. We say $\mathscr{S}$ generates $\mathscr{F}$.
(b) Let $T: M \to N$ where M, N have associated σ-fields $\mathscr{R}$, $\mathscr{F}$. Let $\mathscr{S}$ generate $\mathscr{F}$. Prove T is measurable if and only if $T^{-1}[S] \subset \mathscr{R}$ for all $S \in \mathscr{S}$.

*24. Let μ, ν be two finite measures. Prove ν is a.c.w.r.t. μ if and only if $(\forall \varepsilon)(\exists \delta)\ \mu(A) < \delta$ implies $\nu(A) < \varepsilon$.

25. Consider the function $f(x\ y)$ on $\mathbb{R}^2$ given by

$$f(x, y) = \begin{cases} 1, & x > 0,\ y > 0,\ 0 \leq x - y \leq 1 \\ -1, & x > 0,\ y > 0,\ 0 < y - x \leq 1 \\ 0, & \text{otherwise} \end{cases}$$

Compute $\int_{-\infty}^{\infty} (\int_{-\infty}^{\infty} f(x, y)\, dy)\, dx$ and $\int_{-\infty}^{\infty} (\int_{-\infty}^{\infty} f(x, y)\, dx)\, dy$ and comment on Fubini's theorem and Theorem I.22.

26. Construct a sequence of functions, f_n, which are continuous and pointwise convergent to a function f which is *not* continuous. Prove directly: (a) the convergence $f_n(x) \to f(x)$ is not uniform in x, (b) the f_n are not equicontinuous.

27. Use an $\varepsilon/3$ argument to prove the following: Let B be a complete normed linear space and suppose T_n is a sequence of linear maps $T_n : B \to B$ with two properties: (i) The T_n are bounded uniformly in n, that is, $\|T_n\| \leq C$ for some C independent of n. (ii) For a dense set $D \subset B$, $T_n x$ converges if $x \in D$. Then $T_n x$ converges for each x and the limiting function, Tx, so defined is a bounded linear map.

28. Construct a sequence $f_n(x)$ of bounded functions on $[0, 1]$ converging to zero in L^1 so that f_n converges at no point in $[0, 1]$.

†*29.* Use an $\varepsilon/3$ argument to prove Theorem I.26.

30. A metric space X is called *totally bounded* if for every ε, X can be covered by finitely many ε-balls. Prove that a pointwise convergent uniformly equicontinuous sequence of functions on a totally bounded metric space is uniformly convergent.

31. (a) Using the Heine–Borel property, prove that a continuous function on $[0, 1]$ is uniformly continuous.
(b) Prove that an equicontinuous family of functions on $[0, 1]$ is uniformly equicontinuous.

32. Let $F(x, y)$ be a continuous function on $[0, 1] \times [0, 1]$ and consider the map $\mathscr{F}$: $C[0, 1] \to C[0, 1]$ given by

$$(\mathscr{F}f)(x) = \int_0^1 F(x, y)f(y)\,dy$$

Prove that $\{\mathscr{F}f \mid \|f\|_\infty \leq 1\}$ is an equicontinuous family so that any given sequence f_n with $\|f_n\| \leq 1$, all n, has a subsequence $f_{n(l)}$ with $\mathscr{F}f_{n(l)}$ uniformly convergent.

Remark. It is this last subsequence property that makes $\mathscr{F}$ what is known as a compact operator (a class we discuss in Section VI.5). The classical Fredholm theory of integral equations works because $\mathscr{F}$ is a compact operator.

**33.* (a) Let D be a domain in the complex plane. Let $\mathscr{F}$ be a family of analytic function on D so that, for any compact set $C \subset D$, $\{|f(z)| \mid f \in \mathscr{F}, z \in C\}$ is bounded. Prove that $\mathscr{F}$ is an equicontinuous family by using the Cauchy integral formula.
(b) Prove the Vitali convergence theorem: If D is a connected domain of the complex plane and if f_n is a sequence of analytic functions on D uniformly bounded on compact subsets of D and if $f_n(z)$ converges pointwise for all z lying in some subset of D with a limit point in D, then f_n converges uniformly on compact subsets to an analytic function. (Hint: Use Problem 4.)
(c) Prove Vitali's theorem by a Taylor series and analytic continuation argument.

Remark. For a discussion of Vitali's theorem from the point of view of (c), see E. C. Titchmarsh, *Theory of Functions*, Oxford Univ. Press, London and New York, 1939, pp. 168–170.

II: Hilbert Spaces

Gentlemen: there's lots of room left in Hilbert space — *S. MacLane*

II.1 The geometry of Hilbert space

Finite-dimensional vector spaces have three kinds of properties whose generalizations we will study in the next four chapters: linear properties, metric properties, and geometric properties. In this chapter we study vector spaces that have an inner product, a generalization of the usual dot product on finite dimensional vector spaces. The geometric properties of these spaces follow from the notion of angle which is implicit in the definition of inner product.

Definition A complex vector space V is called an **inner product space** if there is a complex-valued function $(\cdot, \cdot)$ on $V \times V$ that satisfies the following four conditions for all $x, y, z \in V$ and $\alpha \in \mathbb{C}$:

(i) $(x, x) \geq 0$ and $(x, x) = 0$ if and only if $x = 0$
(ii) $(x, y + z) = (x, y) + (x, z)$
(iii) $(x, \alpha y) = \alpha(x, y)$
(iv) $(x, y) = \overline{(y, x)}$

The function $(\cdot, \cdot)$ is called an inner product.

We note that (ii), (iii), and (iv) imply that $(x, \alpha y + \beta z) = \alpha(x, y) + \beta(x, z)$ and that $(\alpha x, y) = \bar{\alpha}(x, y)$. The reader should be aware that some texts use a convention different from the one introduced in (iii); they take the inner product to be linear in the *first* vector and conjugate-linear in the *second.*

Example 1 ($\mathbb{C}^n$) Let $\mathbb{C}^n$ denote the set of all n-tuples of complex numbers. For $x = \langle x_1, \ldots, x_n \rangle$ and $y = \langle y_1, \ldots, y_n \rangle$ in $\mathbb{C}^n$ define

$$(x, y) = \sum_{j=1}^{n} \bar{x}_j y_j$$

Example 2 Let $C[a, b]$ denote the complex-valued continuous functions on the interval $[a, b]$. For $f(x), g(x) \in C[a, b]$ define

$$(f, g) = \int_a^b \overline{f(x)} g(x)\, dx$$

We now develop those geometrical notions that extend to arbitrary inner product spaces.

Definition Two vectors, x and y, in an inner product space V are said to be **orthogonal** if $(x, y) = 0$. A collection $\{x_i\}$ of vectors in V is called an **orthonormal set** if $(x_i, x_i) = 1$ for all i, and $(x_i, x_j) = 0$ if $i \neq j$.

We introduce the shorthand $\|x\| = \sqrt{(x, x)}$. We will shortly see that $\|\cdot\|$ is in fact a norm.

Theorem II.1 (Pythagorean theorem) Let $\{x_n\}_{n=1}^N$ be an orthonormal set in an inner product space V. Then for all $x \in V$,

$$\|x\|^2 = \sum_{n=1}^{N} |(x, x_n)|^2 + \left\| x - \sum_{n=1}^{N} (x_n, x) x_n \right\|^2$$

Proof We write x as

$$x = \sum_{n=1}^{N} (x_n, x) x_n + \left(x - \sum_{n=1}^{N} (x_n, x) x_n \right)$$

A short computation using the properties of inner products shows that

$$\sum_{n=1}^{N} (x_n, x) x_n \quad \text{and} \quad x - \sum_{n=1}^{N} (x_n, x) x_n$$

are orthogonal. Thus,

$$(x, x) = \left\| \sum_{n=1}^{N} (x_n, x)x_n \right\|^2 + \left\| x - \sum_{n=1}^{N} (x_n, x)x_n \right\|^2$$
$$= \sum_{n=1}^{N} |(x_n, x)|^2 + \left\| x - \sum_{n=1}^{N} (x_n, x)x_n \right\|^2 \blacksquare$$

Corollary (Bessel's inequality) Let $\{x_n\}_{n=1}^{N}$ be an orthonormal set in an inner product space, V. Then for all $x \in V$,

$$\|x\|^2 \geq \sum_{n=1}^{N} |(x, x_n)|^2$$

Corollary (the Schwarz inequality) If x and y are vectors in an inner product space V, then

$$|(x, y)| \leq \|x\| \, \|y\|$$

Proof The case $y = 0$ is trivial, so suppose $y \neq 0$. The vector $y/\|y\|$ by itself forms an orthonormal set, so applying Bessel's inequality to any $x \in V$ we get

$$\|x\|^2 \geq |(x, y/\|y\|)|^2 = \frac{|(x, y)|^2}{\|y\|^2}$$

from which $|(x, y)| \leq \|x\| \, \|y\|$ follows. $\blacksquare$

Another useful geometric equality is the parallelogram law (Problem 4):

$$\|x + y\|^2 + \|x - y\|^2 = 2\|x\|^2 + 2\|y\|^2$$

In Section I.2 we defined normed linear spaces and observed that every normed linear space is a metric space. The following theorem shows that every inner product space is a normed linear space.

Theorem II.2 Every inner product space V is a normed linear space with the norm $\|x\| = (x, x)^{1/2}$

Proof Since V is a vector space, we need only verify that $\|\cdot\|$ has all the properties of a norm. All of these properties, except the triangle inequality, follow immediately from the properties (i)–(iv) of inner products. Suppose $x, y \in V$. Then

$$\begin{aligned} \|x + y\|^2 &= (x, x) + (x, y) + (y, x) + (y, y) \\ &= (x, x) + 2 \operatorname{Re}(x, y) + (y, y) \\ &\leq (x, x) + 2|(x, y)| + (y, y) \\ &\leq (x, x) + 2(x, x)^{1/2}(y, y)^{1/2} + (y, y) \end{aligned}$$

Example 3 (ℓ_2) Define ℓ_2 to be the set of sequences $\{x_n\}_{n=1}^{\infty}$ of complex numbers which satisfy $\sum_{n=1}^{\infty} |x_n|^2 < \infty$ with the inner product

$$(\{x_n\}_{n=1}^{\infty}, \{y_n\}_{n=1}^{\infty}) = \sum_{n=1}^{\infty} \bar{x}_n y_n$$

In Section II.3 we will see that any Hilbert space that has a countable dense set and is not finite dimensional is isomorphic to ℓ_2. In this sense, ℓ_2 is the canonical example of a Hilbert space.

Example 4 ($L^2(\mathbb{R}^n, d\mu)$) Let μ be a Borel measure on $\mathbb{R}^n$. $L^2(\mathbb{R}^n, d\mu)$ is the set of complex-valued measurable functions on $\mathbb{R}^n$ which satisfy $\int_{\mathbb{R}^n} |f(x)|^2 \, d\mu < \infty$. $L^2(\mathbb{R}^n, d\mu)$ is a Hilbert space under the inner product

$$(f, g) = \int_{\mathbb{R}^n} \overline{f(x)} g(x) \, d\mu$$

Example 5 (direct sum) Suppose that $\mathscr{H}_1$ and $\mathscr{H}_2$ are Hilbert spaces. Then the set of pairs $\langle x, y \rangle$ with $x \in \mathscr{H}_1$, $y \in \mathscr{H}_2$ is a Hilbert space with inner product

$$(\langle x_1, y_1 \rangle, \langle x_2, y_2 \rangle) = (x_1, x_2)_{\mathscr{H}_1} + (y_1, y_2)_{\mathscr{H}_2}$$

This space is called the **direct sum** of the spaces $\mathscr{H}_1$ and $\mathscr{H}_2$ and is denoted by $\mathscr{H}_1 \oplus \mathscr{H}_2$. If μ_1 and μ_2 are mutually singular Borel measures on $\mathbb{R}$ and $\mu = \mu_1 + \mu_2$, then $L^2(\mathbb{R}, d\mu)$ is isomorphic in a natural way to $L^2(\mathbb{R}, d\mu_1) \oplus L^2(\mathbb{R}, d\mu_2)$ (Problem 3). We can also construct countable direct sums as follows. Suppose $\{\mathscr{H}_n\}_{n=1}^{\infty}$ is a sequence of Hilbert spaces. Let $\mathscr{H}$ denote the set of sequences $\{x_n\}_{n=1}^{\infty}$, with $x_n \in \mathscr{H}_n$, which satisfy

$$\sum_{n=1}^{\infty} \|x_n\|_{\mathscr{H}_n}^2 < \infty$$

$\mathscr{H}$ is a Hilbert space under the natural inner product and is denoted by

$$\mathscr{H} = \bigoplus_{n=1}^{\infty} \mathscr{H}_n$$

Example 6 (vector-valued functions) Suppose $\langle X, \mu \rangle$ is a measure space and $\mathscr{H}'$ is a Hilbert space. Let $L^2(X, d\mu; \mathscr{H}')$ be the set of measurable functions on X with values in $\mathscr{H}'$ which satisfy

$$\int \|f(x)\|_{\mathscr{H}'}^2 \, d\mu(x) < \infty$$

by the Schwarz inequality. Thus

$$\|x + y\|^2 \leq (\|x\| + \|y\|)^2$$

which proves the triangle inequality. ∎

This theorem shows that we have a natural metric,

$$d(x, y) = \sqrt{(x - y, x - y)}$$

in V. We thus have the notions of convergence, completeness, and density defined for metric spaces in Section I.2. In particular, we can always complete V to a normed linear space $\tilde{V}$ in which V is isometrically embedded as a dense subset. In fact, $\tilde{V}$ is also an inner product space since the inner product can be extended from V to $\tilde{V}$ by continuity (Problem 1).

Definition A complete inner product space is called a **Hilbert space**. Inner product spaces are sometimes called pre-Hilbert spaces.

Definition Two Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$ are said to be **isomorphic** if there is a linear operator U from $\mathscr{H}_1$ *onto* $\mathscr{H}_2$ such that $(Ux, Uy)_{\mathscr{H}_2} = (x, y)_{\mathscr{H}_1}$ for all $x, y \in \mathscr{H}_1$. Such an operator is called **unitary**.

We elaborate these ideas and show the reader what types of Hilbert spaces he is likely to meet by a series of examples.

Example 2 (revisited) Define $L^2[a, b]$ to be the set of complex-valued measurable functions on $[a, b]$, a finite interval, that satisfy $\int_a^b |f(x)|^2\, dx < \infty$. We define an inner product by

$$(f, g) = \int_a^b \overline{f(x)} g(x)\, dx$$

Observe that the inner makes sense since

$$|\overline{f(x)} g(x)| \leq \tfrac{1}{2}|f(x)|^2 + \tfrac{1}{2}|g(x)|^2$$

so that $\overline{f(x)} g(x)$ is in $L^1[a, b]$. A proof similar to the Riesz–Fisher theorem (Theorem I.12) shows that $L^2[a, b]$ is complete and is therefore a Hilbert space. It is not too difficult to show (Problem 2) that $L^2[a, b]$ is the completion of $C[a, b]$ in the norm

$$\|f\| = \left(\int_a^b |f(x)|^2\, dx\right)^{1/2}$$

This set is a Hilbert space with the inner product

$$(f, g) = \int_X (f(x), g(x))_{\mathscr{H}} \, d\mu(x)$$

Of course, we have not said what it means for a vector-valued function to be measurable. For this definition and related matters see Problem 12 and the appendix to Section IV.5.

II.2 The Riesz lemma †

In the examples in Section II.1 we showed several ways of constructing new Hilbert spaces from old ones. Another way to do this is to restrict attention to a closed subspace $\mathscr{M}$ of the given Hilbert space $\mathscr{H}$. Under the natural inner product that it inherits as a subspace of $\mathscr{H}$, $\mathscr{M}$ is a Hilbert space. We denote by $\mathscr{M}^\perp$ the set of vectors in $\mathscr{H}$ which are orthogonal to $\mathscr{M}$; $\mathscr{M}^\perp$ is called the **orthogonal complement** of $\mathscr{M}$. It follows from the linearity of the inner product that $\mathscr{M}^\perp$ is a linear subspace of $\mathscr{H}$ and an elementary argument (Problem 6) shows that $\mathscr{M}^\perp$ is closed. Thus $\mathscr{M}^\perp$ is also a Hilbert space. $\mathscr{M}$ and $\mathscr{M}^\perp$ have only the zero element in common. The following theorem shows that there are vectors perpendicular to any closed proper subspace, indeed there are enough of them so that

$$\mathscr{H} = \mathscr{M} + \mathscr{M}^\perp = \{x + y \,|\, x \in \mathscr{M}, y \in \mathscr{M}^\perp\}$$

This important geometric property is one of the main reasons that Hilbert spaces are easier to handle than Banach spaces (Chapter III). In the following lemma and theorem, the reader should keep the finite-dimensional case in mind (see Figure II.1).

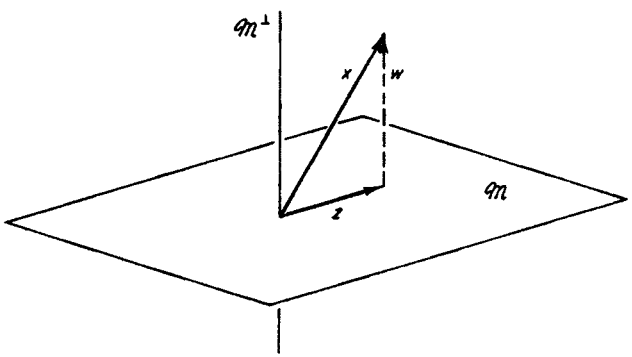

FIGURE II.1 The projection of x on $\mathscr{M}$.

† A supplement to this section begins on p. 344.

Lemma Let $\mathscr{H}$ be a Hilbert space, $\mathscr{M}$ a closed subspace of $\mathscr{H}$, and suppose $x \in \mathscr{H}$. Then there exists in $\mathscr{M}$ a unique element z closest to x.

Proof Let $d = \inf_{y \in \mathscr{M}} \|x - y\|$. Choose a sequence $\{y_n\}$, $y_n \in \mathscr{M}$, so that

$$\|x - y_n\| \to d$$

Then

$$\begin{aligned}
\|y_n - y_m\|^2 &= \|(y_n - x) - (y_m - x)\|^2 \\
&= 2\|y_n - x\|^2 + 2\|y_m - x\|^2 - \|-2x + y_n + y_m\|^2 \\
&= 2\|y_n - x\|^2 + 2\|y_m - x\|^2 - 4\|x - \tfrac{1}{2}(y_n + y_m)\|^2 \\
&\leq 2\|y_n - x\|^2 + 2\|y_m - x\|^2 - 4d^2 \\
&\underset{\substack{m \to \infty \\ n \to \infty}}{\longrightarrow} 2d^2 + 2d^2 - 4d^2 = 0
\end{aligned}$$

The second equality follows from the parallelogram law; the inequality follows from the fact that $\frac{1}{2}(y_n + y_m) \in \mathscr{M}$. Thus $\{y_n\}$ is Cauchy and since $\mathscr{M}$ is closed, $\{y_n\}$ converges to an element z of $\mathscr{M}$. It follows easily that $\|x - z\| = d$. Uniqueness is left as an exercise. ∎

Theorem II.3 (the projection theorem) Let $\mathscr{H}$ be a Hilbert space, $\mathscr{M}$ a closed subspace. Then every $x \in \mathscr{H}$ can be uniquely written $x = z + w$ where $z \in \mathscr{M}$ and $w \in \mathscr{M}^\perp$.

Proof Let x be in $\mathscr{H}$. Then by the lemma there is a unique element $z \in \mathscr{M}$ closest to x. Define $w = x - z$, then we clearly have $x = z + w$. Let $y \in \mathscr{M}$ and $t \in \mathbb{R}$. If $d = \|x - z\|$, then

$$\begin{aligned}
d^2 \leq \|x - (z + ty)\|^2 &= \|w - ty\|^2 \\
&= d^2 - 2t\,\mathrm{Re}(w, y) + t^2\|y\|^2
\end{aligned}$$

Thus, $-2t\,\mathrm{Re}(w, y) + t^2\|y\|^2 \geq 0$ for all t, which implies $\mathrm{Re}(w, y) = 0$. A similar argument using ti instead of t shows that $\mathrm{Im}(w, y) = 0$. Thus, $w \in \mathscr{M}^\perp$. Uniqueness is left as an exercise. ∎

The projection theorem sets up a natural isomorphism between $\mathscr{M} \oplus \mathscr{M}^\perp$ and $\mathscr{H}$ given by

$$\langle z, w \rangle \mapsto z + w$$

We will often suppress the isomorphism and simply write $\mathscr{H} = \mathscr{M} \oplus \mathscr{M}^\perp$.

We have already defined in Section I.2 what we mean by a bounded linear transformation from one Hilbert space $\mathscr{H}$ to another $\mathscr{H}'$. We will denote by

$\mathscr{L}(\mathscr{H}, \mathscr{H}')$ the set of such transformations. $\mathscr{L}(\mathscr{H}, \mathscr{H}')$ is clearly a vector space and it becomes a Banach space under the norm

$$\|T\| = \sup_{\|x\|_{\mathscr{H}}=1} \|Tx\|_{\mathscr{H}'}.$$

The proof of this fact, though not difficult, is postponed until Chapter III where it is proven in greater generality. For the time being we are interested in the special case where $\mathscr{H}' = \mathbb{C}$:

Definition The space $\mathscr{L}(\mathscr{H}, \mathbb{C})$ is called the **dual space** of $\mathscr{H}$ and is denoted by $\mathscr{H}^*$. The elements of $\mathscr{H}^*$ are called **continuous linear functionals**.

The following important theorem which characterizes $\mathscr{H}^*$ is due to F. Riesz and M. Fréchet.

Theorem II.4 (the Riesz lemma) For each $T \in \mathscr{H}^*$, there is a unique $y_T \in \mathscr{H}$ such that $T(x) = (y_T, x)$ for all $x \in \mathscr{H}$. In addition $\|y_T\|_{\mathscr{H}} = \|T\|_{\mathscr{H}^*}$.

Proof Let $\mathscr{N}$ be the set of $x \in \mathscr{H}$ such that $T(x) = 0$. By the continuity of T, $\mathscr{N}$ is a closed subspace. If $\mathscr{N} = \mathscr{H}$, then $T(x) = 0 = (0, x)$ for all x and we are finished; so assume $\mathscr{N}$ is not all of $\mathscr{H}$. Then by the projection theorem there is a nonzero vector x_0 in $\mathscr{N}^\perp$. Define $y_T = \overline{T(x_0)}\|x_0\|^{-2}x_0$. We will verify that the vector y_T has the right properties. First, if $x \in \mathscr{N}$, then $T(x) = 0 = (y_T, x)$. Further, if $x = \alpha x_0$, then

$$T(x) = T(\alpha x_0) = \alpha T(x_0) = \overline{T(x_0)}\|x_0\|^{-2}x_0, \alpha x_0) = (y_T, \alpha x_0)$$

Since the functions $T(\cdot)$ and $(y_T, \cdot)$ are linear and agree on $\mathscr{N}$ and x_0, they must agree on the space spanned by $\mathscr{N}$ and x_0. But $\mathscr{N}$ and x_0 span $\mathscr{H}$ since every element $y \in \mathscr{H}$ can be written

$$y = \left(y - \frac{T(y)}{T(x_0)}x_0\right) + \frac{T(y)}{T(x_0)}x_0$$

Thus $T(x) = (y_T, x)$ for all $x \in \mathscr{H}$. If $T(x) = (y', x)$ also, then $\|y' - y_T\|^2 = T(y' - y_T) - T(y' - y_T) = 0$ so $y' = y_T$, proving uniqueness.

To prove that $\|T\|_{\mathscr{H}^*} = \|y_T\|_{\mathscr{H}}$ we observe that

$$\|T\| = \sup_{\|x\| \le 1} |T(x)| = \sup_{\|x\| \le 1} |(y_T, x)| \le \sup_{\|x\| \le 1} \|y_T\| \|x\| = \|y_T\|$$

and

$$\|T\| = \sup_{\|x\| \le 1} |T(x)| \ge \left|T\left(\frac{y_T}{\|y_T\|}\right)\right| = \left(y_T, \frac{y_T}{\|y_T\|}\right) = \|y_T\| \quad \blacksquare$$

We note that the Schwarz inequality shows that the converse of the Riesz lemma is true. Namely, each $y \in \mathscr{H}$ defines a continuous linear functional T_y on $\mathscr{H}$ by $T_y(x) = (y, x)$. The Riesz lemma has the following corollary which is very important in applications.

Corollary Let $B(\cdot, \cdot)$ be a function from $\mathscr{H} \times \mathscr{H}$ to $\mathbb{C}$ which satisfies:

(i) $B(x, \alpha y + \beta z) = \alpha B(x, y) + \beta B(x, z)$
(ii) $B(\alpha x + \beta y, z) = \bar{\alpha} B(x, z) + \bar{\beta} B(y, z)$
(iii) $|B(x, y)| \leq C\|x\| \, \|y\|$

for all $x, y, z \in \mathscr{H}$, $\alpha, \beta \in \mathbb{C}$. Then there is a unique bounded linear transformation A, from $\mathscr{H}$ to $\mathscr{H}$ so that

$$B(x, y) = (Ax, y) \qquad \text{for all} \quad x, y \in \mathscr{H}$$

The norm of A is the smallest constant C such that (iii) holds.

Proof Fix x, then (i) and (iii) show that $B(x, \cdot)$ is a continuous linear functional on $\mathscr{H}$. Thus by the Riesz lemma there is an $x' \in \mathscr{H}$ so that

$$B(x, y) = (x', y) \qquad \text{for all} \quad y \in \mathscr{H}$$

Define $Ax = x'$. It is not difficult to show that A is a continuous linear operator with the right properties (Problem 8). ∎

A bilinear function on $\mathscr{H}$ obeying (i) and (ii) is called a **sesquilinear form**.

II.3 Orthonormal bases

We have already defined what it means for a set of vectors to be orthonormal. In this section we develop this idea further; in particular we want to extend the idea of a "basis," so useful for finite-dimensional vector spaces, to complete inner product spaces. If S is an orthonormal set in a Hilbert space $\mathscr{H}$ and no other orthonormal set contains S as a proper subset, then S is called an **orthonormal basis** (or a **complete orthonormal system**) for $\mathscr{H}$.

Theorem II.5 Every Hilbert space $\mathscr{H}$ has an orthonormal basis.

Proof Consider the collection $\mathscr{C}$ of orthonormal sets in V. We order $\mathscr{C}$ by inclusion; that is, we say $S_1 \prec S_2$ if $S_1 \subset S_2$. With this definition of $\prec$, $\mathscr{C}$ is partially ordered; it is also nonempty since if v is any element of V, the

set consisting only of $v/\|v\|$ is an orthonormal set. Now let $\{S_\alpha\}_{\alpha\in A}$ be any linearly ordered subset of $\mathscr{C}$. Then $\bigcup_{\alpha\in A} S_\alpha$ is an orthonormal set which contains each S_α and is thus an upper bound for $\{S_\alpha\}_{\alpha\in A}$. Since every linearly ordered subset of $\mathscr{C}$ has an upper bound, we can apply Zorn's lemma (Theorem I.2) and conclude that $\mathscr{C}$ has a maximal element; that is, an orthonormal system not properly contained in any other orthonormal system. ∎

The following theorem shows that as in the finite-dimensional case every element of a Hilbert space can be expressed as a linear combination (possibly infinite) of basis elements.

Theorem II.6 Let $\mathscr{H}$ be a Hilbert space and $S = \{x_\alpha\}_{\alpha\in A}$ an orthonormal basis. Then for each $y \in \mathscr{H}$,

$$y = \sum_{\alpha\in A} (x_\alpha, y)x_\alpha \tag{II.1}$$

and

$$\|y\|^2 = \sum_{\alpha\in A} |(x_\alpha, y)|^2 \tag{II.2}$$

The equality in (II.1) means that the sum on the right-hand side converges (independent of order) to y in $\mathscr{H}$. Conversely, if $\sum_{\alpha\in A} |c_\alpha|^2 < \infty$, $c_\alpha \in \mathbb{C}$, then $\sum_{\alpha\in A} c_\alpha x_\alpha$ converges to an element of $\mathscr{H}$.

Proof We have already shown in Section II.1 (Bessel's inequality) that for any finite subset $A' \subset A$, $\sum_{\alpha\in A'} |(x_\alpha, y)|^2 \le \|y\|^2$. Thus $(x_\alpha, y) \neq 0$ for at most a countable number of α's in A which we order in some way $\alpha_1, \alpha_2, \alpha_3, \ldots$. Furthermore, since $\sum_{j=1}^{N} |(x_{\alpha_j}, y)|^2$ is monotone increasing and bounded, it converges to a finite limit as $N \to \infty$. Let $y_n = \sum_{j=1}^{n} (x_{\alpha_j}, y)x_{\alpha_j}$. Then for $n > m$,

$$\|y_n - y_m\|^2 = \left\| \sum_{j=m+1}^{n} (x_{\alpha_j}, y)x_{\alpha_j} \right\|^2 = \sum_{j=m+1}^{n} |(x_{\alpha_j}, y)|^2$$

Therefore $\{y_n\}$ is a Cauchy sequence and converges to an element y' of $\mathscr{H}$. Observe that

$$\begin{aligned}(y - y', x_{\alpha_\ell}) &= \lim_{n\to\infty} \left(y - \sum_{j=1}^{n} (x_{\alpha_j}, y)x_{\alpha_j}, x_{\alpha_\ell} \right) \\ &= (y, x_{\alpha_\ell}) - (y, x_{\alpha_\ell}) = 0\end{aligned}$$

And if $\alpha \neq \alpha_\ell$ for some ℓ we have

$$(y - y', x_\alpha) = \lim_{n\to\infty} \left(y - \sum_{j=1}^{n} (x_{\alpha_j}, y)x_{\alpha_j}, x_\alpha \right) = 0$$

Therefore $y - y'$ is orthogonal to all the x_α in S. Since S is a complete orthonormal system we must have $y - y' = 0$. Thus

$$y = \lim_{n\to\infty} \sum_{j=1}^{n} (x_{\alpha_j}, y)x_{\alpha_j}$$

and (II.1) holds. Furthermore,

$$\begin{aligned} 0 &= \lim_{n\to\infty} \left\| y - \sum_{j=1}^{n} (x_{\alpha_j}, y)x_{\alpha_j} \right\|^2 \\ &= \lim_{n\to\infty} \left(\|y\|^2 - \sum_{j=1}^{n} |(x_{\alpha_j}, y)|^2 \right) \\ &= \|y\|^2 - \sum_{\alpha\in A} |(x_\alpha, y)|^2 \end{aligned}$$

so that (II.2) holds also. We omit the easy proof of the converse statement. ∎

We note that (II.2) is called Parseval's relation. The coefficients (x_α, y) are often called the **Fourier coefficients** of y with respect to the basis $\{x_\alpha\}$. The reason for this terminology will become apparent shortly.

We now describe a useful procedure, called Gram–Schmidt orthogonalization, for constructing an orthonormal set from an arbitrary sequence of independent vectors. Suppose the independent vectors $u_1, u_2, \ldots$ are given and define

$$\begin{aligned} w_1 &= u_1, & v_1 &= w_1/\|w_1\| \\ w_2 &= u_2 - (v_1, u_1)v_k, & v_2 &= w_2/\|w_2\| \\ &\vdots & &\vdots \\ w_n &= u_n - \sum_{k=1}^{n-1} (v_k, u_n)v_k, & v_n &= w_n/\|w_n\| \\ &\vdots & &\vdots \end{aligned}$$

The family $\{v_j\}$ is an orthonormal set and has the property that for each m, $\{u_j\}_{j=1}^m$ and $\{v_j\}_{j=1}^m$ span the same vector space. In particular, the set of finite linear combinations of all the v's is the same as the finite linear combinations of the u's (see Figure II.2).

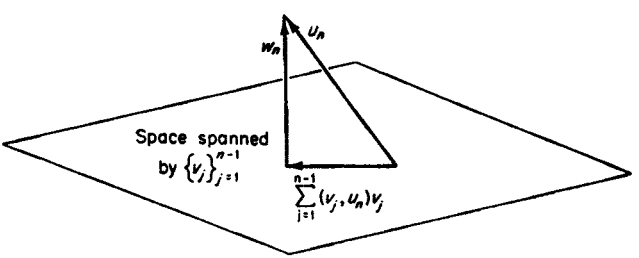

FIGURE II.2 Gram–Schmidt orthogonalization.

We remark that the Legendre polynomials (up to constant multiples) are obtained by applying the Gram–Schmidt process to the functions 1, x, x^2, x^3, ..., on the interval $[-1, 1]$ with the usual L^2 inner product.

Definition A metric space which has a countable dense subset is said to be **separable.**

Most Hilbert spaces that arise in practice are separable. The following theorem characterizes them up to isomorphism.

Theorem II.7 A Hilbert space $\mathscr{H}$ is separable if and only if it has a countable orthonormal basis S. If there are $N < \infty$ elements in S, then $\mathscr{H}$ is isomorphic to $\mathbb{C}^N$. If there are countably many elements in S, then $\mathscr{H}$ is isomorphic to ℓ_2 (Example 3, Section II.1).

Proof Suppose $\mathscr{H}$ is separable and let $\{x_n\}$ be a countable dense set. By throwing out some of the x_n's we can get a subcollection of independent vectors whose span (finite linear combinations) is the same as the $\{x_n\}$ and is thus dense. Applying the Gram–Schmidt procedure to this subcollection we obtain a countable complete orthonormal system. Conversely, if $\{y_n\}$ is a complete orthonormal system for a Hilbert space $\mathscr{H}$ then it follows from Theorem II.6 that the set of finite linear combinations of the y_n with rational coefficients is dense in $\mathscr{H}$. Since this set is countable, $\mathscr{H}$ is separable.

Suppose $\mathscr{H}$ is separable and $\{y_n\}_{n=1}^{\infty}$ is a complete orthonormal system. We define a map $\mathscr{U}: \mathscr{H} \to \ell_2$ by

$$\mathscr{U}: x \to \{(y_n, x)\}_{n=1}^{\infty}$$

Theorem II.6 shows that this map is well defined and onto. It is easy to show it is unitary. The proof that $\mathscr{H}$ is isomorphic to $\mathbb{C}^N$ if S has N elements is similar. ∎

Notice that in the separable case, the Gram–Schmidt process allows us to construct an orthonormal basis without using Zorn's lemma.

We conclude this section with an example that shows how Hilbert spaces arose naturally from problems in classical analysis. If $f(x)$ is an integrable function on $[0, 2\pi]$ we can define the numbers

$$c_n = \frac{1}{(2\pi)^{1/2}} \int_0^{2\pi} e^{-inx} f(x)\, dx$$

The formal series $\sum_{n=-\infty}^{\infty} c_n (2\pi)^{-1/2} e^{inx}$ is called the Fourier series of f. The classical problem is: for which f and in what sense does the Fourier series of

f converge to f? This problem which originated with Fourier in 1811 has hac a rich and eventful history. It has given rise to an entire branch of modern mathematics (abstract harmonic analysis). Furthermore, some of the nices results on the classical case have just been proven recently (see the Notes). As an example of a classical result we state (Problems 14 and 15):

Theorem II.8 Suppose that $f(x)$ is periodic of period 2π and is continuously differentiable. Then the functions $\sum_{-M}^{M} c_n e^{inx}$ converge uniformly to $f(x)$ as $M \to \infty$.

This theorem gives sufficient conditions for the Fourier series of a function to converge uniformly. But, finding the exact class of functions whose Fourier series converge uniformly or converge pointwise has proved to be a hard problem. We can, however, get a nice answer to this question if we change our notion of "convergence" and this is just where Hilbert spaces come in. The collection of functions, $\{(2\pi)^{-1/2} e^{inx}\}_{-\infty}^{\infty}$, is clearly an orthonormal set in $L^2[0, 2\pi]$. If we knew that it was a *complete* orthonormal set, then Theorem II.6 would allow us to conclude that for all functions in $L^2[0, 2\pi]$,

$$f(x) = \lim_{M \to \infty} \sum_{-M}^{M} (2\pi)^{-1/2} c_n e^{inx}$$

where convergence means convergence in the L^2 norm. In fact, $\{(2\pi)^{-1/2} e^{inx}\}_{-\infty}^{\infty}$ is complete. We will give a proof that relies on the classical theorem stated above.

Theorem II.9 If $f \in L^2[0, 2\pi]$, then $\sum_{-M}^{M} c_n (2\pi)^{-1/2} e^{inx}$ converges to f in the L^2 norm as $M \to \infty$.

Proof We need to know that the periodic, continuously differentiable functions $C_p^1[0, 2\pi]$ are dense in $L^2[0, 2\pi]$. In Problem 2 the reader is asked to show that the step functions are dense. But a step function can be approximated (in L^2) by a $C_p^1[0, 2\pi]$ function by rounding off the corners in a smooth way and by changing it at one end to make it periodic. The reader should convince himself that this can be done so that the resulting function is arbitrarily close to the step function in L^2 norm.

To show that $\{(2\pi)^{-1/2} e^{inx}\}_{-\infty}^{\infty}$ is a complete set we need only show that $(e^{inx}, g) = 0$ for all n implies $g = 0$. Suppose $f \in C_p^1[0, 2\pi]$, then by Theorem II.8

$$\sum_{-M}^{M} c_n (2\pi)^{-1/2} e^{inx} \to f$$

uniformly and thus in the L^2 sense also. Therefore,

$$(f, g) = \lim_{M \to \infty} \left(\sum_{-M}^{M} c_n (2\pi)^{-1/2} e^{inx}, g \right) = 0$$

if $(e^{inx}, g) = 0$ for all n. But, then g is orthogonal to all f in the dense set $C_p^1[0, 2\pi]$ which implies $g = 0$. Thus $\{(2\pi)^{-1/2} e^{inx}\}_{-\infty}^{\infty}$ is a complete orthonormal set, and it follows from Theorem II.6 that the Fourier series of every $L^2[0, 2\pi]$ function converges in the L^2-norm to the function. ∎

This theorem shows that the "natural" notion of convergence for Fourier series is L^2 convergence and illustrates one of the basic principles of functional analysis: namely, to choose an abstract space and a notion of convergence that is appropriate to the problem at hand, a space in which one can prove nice theorems. By doing this one avoids some hard problems; this has both advantages and disadvantages.

II.4 Tensor products of Hilbert spaces

We described in Sections II.1 and II.2 several ways of making new Hilbert spaces from old ones. In this section we describe the tensor product $\mathscr{H}_1 \otimes \mathscr{H}_2$ of two Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. The construction of the tensor product which we use is not the most elegant, but is very direct. The reader can easily extend our proofs to construct the tensor product $\mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_n$ of finitely many Hilbert spaces.

Let $\mathscr{H}_1$ and $\mathscr{H}_2$ be Hilbert spaces. For each $\varphi_1 \in \mathscr{H}_1$, $\varphi_2 \in \mathscr{H}_2$, let $\varphi_1 \otimes \varphi_2$ denote the conjugate bilinear form which acts on $\mathscr{H}_1 \times \mathscr{H}_2$ by

$$(\varphi_1 \otimes \varphi_2)\langle \psi_1, \psi_2 \rangle = (\psi_1, \varphi_1)(\psi_2, \varphi_2)$$

Let $\mathscr{E}$ be the set of finite linear combinations of such conjugate linear forms; we define an inner product $(\cdot, \cdot)$ on $\mathscr{E}$ by defining

$$(\varphi \otimes \psi, \eta \otimes \mu) = (\varphi, \eta)(\psi, \mu)$$

and extending by linearity to $\mathscr{E}$.

Proposition 1 $(\cdot, \cdot)$ is well defined and positive definite.

Proof To show that $(\cdot, \cdot)$ is well defined, we must show that (λ, λ') does not depend on which finite linear combinations are used to express λ and λ'. To

do this it is sufficient to show that if μ is a finite sum which is the zero form, then $(\eta, \mu) = 0$ for all $\eta \in \mathscr{E}$. To see that this is true, let $\eta = \sum_{i=1}^{N} c_i(\varphi_i \otimes \psi_i)$, then

$$\begin{aligned}(\eta, \mu) &= \left(\sum_{i=1}^{N} c_i(\varphi_i \otimes \psi_i), \mu\right) \\ &= \sum_{i=1}^{N} c_i \mu\langle \varphi_i, \psi_i\rangle \\ &= 0\end{aligned}$$

since μ is the zero form. Thus, $(\cdot, \cdot)$ is well defined.

Now, suppose $\lambda = \sum_{k=1}^{M} d_k(\eta_k \otimes \mu_k)$. Then $\{\eta_k\}_{k=1}^{M}$ and $\{\mu_k\}_{k=1}^{M}$ span subspaces $M_1 \subset \mathscr{H}_1$ and $M_2 \subset \mathscr{H}_2$ respectively. If we let $\{\varphi_j\}_{j=1}^{N_1}$ and $\{\psi_\ell\}_{\ell=1}^{N_2}$ be orthonormal bases for M_1 and M_2, we can express each η_k in terms of the φ_j's and each μ_k in terms of the ψ_ℓ's obtaining

$$\lambda = \sum_{\substack{j=1 \\ \ell=1}}^{M_1, M_2} c_{j\ell}(\varphi_j \otimes \psi_\ell)$$

But,

$$\begin{aligned}(\lambda, \lambda) &= \left(\sum c_{j\ell}(\varphi_j \otimes \psi_\ell), \sum c_{im}(\varphi_i \otimes \psi_m)\right) \\ &= \sum \overline{c_{j\ell}} c_{im}(\varphi_j, \varphi_i)(\psi_\ell, \psi_m) \\ &= \sum_{j\ell} |c_{j\ell}|^2\end{aligned}$$

so if $(\lambda, \lambda) = 0$, then all the $c_{j\ell} = 0$ and λ is the zero form. Thus $(\cdot, \cdot)$ is positive definite. ∎

Definition We define $\mathscr{H}_1 \otimes \mathscr{H}_2$ to be the completion of $\mathscr{E}$ under the inner product $(\cdot, \cdot)$ defined above. $\mathscr{H}_1 \otimes \mathscr{H}_2$ is called the **tensor product** of $\mathscr{H}_1$ and $\mathscr{H}_2$.

Proposition 2 If $\{\varphi_k\}$ and $\{\psi_\ell\}$ are orthonormal bases for $\mathscr{H}_1$ and $\mathscr{H}_2$ respectively, then $\{\varphi_k \otimes \psi_\ell\}$ is an orthonormal basis for $\mathscr{H}_1 \otimes \mathscr{H}_2$.

Proof To simplify notation, we consider the case in which both $\mathscr{H}_1$ and $\mathscr{H}_2$ are infinite dimensional and separable. The other cases are similar. The set $\{\varphi_k \otimes \psi_\ell\}$ is clearly orthonormal and therefore we need only show that $\mathscr{E}$ is contained in the closed space S spanned by $\{\varphi_k \otimes \psi_\ell\}$. Let $\varphi \otimes \psi \in \mathscr{E}$. Since $\{\varphi_k\}$ and $\{\psi_\ell\}$ are bases, $\varphi = \sum c_k \varphi_k$ and $\psi = \sum d_\ell \psi_\ell$ where $\sum |c_k|^2 < \infty$ and $\sum |d_\ell|^2 < \infty$. Thus $\sum_{k,\ell} |c_k d_\ell|^2 < \infty$. Therefore by Theorem II.6, there

is a vector $\mu = \sum_{k,\ell} c_k d_\ell \varphi_k \otimes \psi_\ell$ in S. By direct computation

$$\|\varphi \otimes \psi - \sum_{\substack{k<M \\ \ell<N}} c_k d_\ell \varphi_k \otimes \psi_\ell\| \to 0$$

as $M, N \to \infty$. ∎

To show how the tensor product arises naturally, we will show how it is related to Hilbert spaces with which the reader is already familiar. First, let $\langle M_1, \mu_1 \rangle$ and $\langle M_2, \mu_2 \rangle$ be measure spaces. We suppose that $L^2(M_1, d\mu_1)$ and $L^2(M_2, d\mu_2)$ are separable (see Problems 24 and 25 of this chapter and Problem 43 of Chapter IV). Let $\{\varphi_k(x)\}$ and $\{\psi_\ell(y)\}$ be bases for $L^2(M_1, d\mu_1)$ and $L^2(M_2, d\mu_2)$ respectively. Then $\{\varphi_k(x)\psi_\ell(y)\}$ is certainly an orthonormal set in $L^2(M_1 \times M_2, d\mu_1 \otimes d\mu_2)$. The fact that $\{\varphi_k(x)\psi_\ell(y)\}$ is actually a basis can be seen as follows. Suppose that $f(x, y) \in L^2(M_1 \times M_2, d\mu_1 \otimes d\mu_2)$, and

$$\iint_{M_1 \times M_2} \overline{f(x, y)} \varphi_k(x) \psi_\ell(y)\, d\mu_1(x)\, d\mu_2(y) = 0$$

for all k and ℓ. By Fubini's theorem this can be rewritten

$$\int_{M_2} \left(\int_{M_1} \overline{f(x, y)} \varphi_k(x)\, d\mu_1(x) \right) \psi_\ell(y)\, d\mu_2(y) = 0$$

Since $\{\psi_\ell\}$ is a basis for $L^2(M_2, \mu_2)$, this implies that

$$\int_{M_1} \overline{f(x, y)} \varphi_k(x)\, d\mu_1(x) = 0$$

except on a set $S_k \subset M_2$ with $\mu_2(S_k) = 0$. Thus, for $y \notin \bigcup S_k$, $\int_{M_1} f(x, y) \times \varphi_k(x)\, d\mu_1(x) = 0$ for all k, which implies that $f(x, y) = 0$, a.e. $[\mu_1]$. Thus, $f(x, y) = 0$ a.e. $[\mu_1 \otimes \mu_2]$. So, $\{\varphi_k(x)\psi_\ell(y)\}$ is a basis for

$$L^2(M_1 \times M_2, d\mu_1 \otimes d\mu_2)$$

Now, let

$$U: \varphi_k \otimes \psi_\ell \to \varphi_k(x)\psi_\ell(y)$$

Then U takes an orthonormal basis for $L^2(M_1, d\mu_1) \otimes L^2(M_2, d\mu_2)$ onto an orthonormal basis for $L^2(M_1 \times M_2, d\mu_1 \otimes d\mu_2)$ and extends uniquely to a unitary mapping of

$$L^2(M_1, d\mu_1) \otimes L^2(M_2, d\mu) \quad \text{onto} \quad L^2(M_1 \times M_2, d\mu_1 \otimes d\mu_2).$$

Let $\varepsilon(\cdot)$ be the function from P_n to $\{1, -1\}$ which is one on even permutations and minus one on odd permutations. Define $A_n = (1/n!) \sum_{\sigma \in \mathcal{P}_n} \varepsilon(\sigma)\sigma$; then A is an orthogonal projection on $\mathcal{H}^n$. $A_n \mathcal{H}^n$ is called the n-fold antisymmetric tensor product of $\mathcal{H}$. In the case where $\mathcal{H} = L^2(\mathbb{R})$, $A_n \mathcal{H}^n$ is just the subspace of $L^2(\mathbb{R}^n)$ consisting of those functions odd under interchange of two coordinates. The subspace

$$\mathcal{F}_a(\mathcal{H}) = \bigoplus_{n=0}^{\infty} A_n \mathcal{H}^n$$

is called the **antisymmetric Fock space over** $\mathcal{H}$ or the **Fermion Fock space over** $\mathcal{H}$.

II.5 Ergodic theory: an introduction

In this section we give a brief introduction to ergodic theory. For our discussion we need several concepts not formally defined until Chapter VI: adjoint operators, projection operators, and the kernel and range of an operator. Any reader not already familiar with these concepts should consult Chapter VI. We give this discussion here because ergodic theory illustrates nicely the power and limitations of Hilbert-space methods and serves as a nice example of the main theme of these books, namely the interplay between functional analysis and mathematical physics. We will see that it is useful to reformulate the question of why macroscopic systems approach equilibrium in terms of abstract spaces, but that one must pay a price: The natural question in the abstract setting is slightly different from the original question and one may be tempted to accept weaker results.

The statement "any system approaches an equilibrium state" is sometimes known as the zeroth law of thermodynamics. From a microscopic point of view it is perhaps surprising that any system should approach equilibrium since microscopically there is no steady state and therefore no equilibrium. Nevertheless, any attempt at a microscopic justification of thermodynamics must explain why the zeroth laws holds macroscopically. There is far from universal agreement among physicists as to what constitutes a justification of the zeroth law, but we would like to avoid a discussion of the pros and cons of the many different approaches which have been suggested (however, see the Notes). The approach that we use is generally accepted by most physicists.

The first basic idea is that thermodynamical systems undergo fluctuations (see Problem 17); put differently, by their very nature the laws of thermo-

dynamics are not absolute statements about a system at a fixed time but are statements about measurements made over time periods long with respect to some characteristic times such as relaxation or collision times. Thus, thermodynamics deals with average measurements of observables over a time period T. Since the collision times, etc., are dependent on the dynamics, one can only hope to prove thermodynamic statements about the limit as $T \to \infty$. How large T has to be for the average over the interval T to be approximately equal to the limit is a detailed dynamical question, but in specific cases one would hope to be able to prove something.

Let us suppose that we describe the state of a classical mechanical system by a point in some phase space Γ. For each time t; there is a map $T_t: \Gamma \to \Gamma$, where $T_t x$ is the state which results by taking a state x at t_0 and waiting until $t_0 + t$ (we are assuming time-translation invariance so t_0 never enters). Obviously, $T_{t+s} = T_t T_s$. In classical mechanics, the observables of the system like energy or angular momentum are functions on phase space. So, our discussion above suggests that we study

$$\lim_{T\to\infty} (1/T) \int_0^T f(T_t x)\, dt$$

We would like to show that the limit exists, at least for continuous functions. Typically Γ is a metric space, so "continuous" has a meaning. Not only would we like the limit to exist, but it should be independent of the initial point x or at least only dependent on a few "macroscopic" observables we can associate with an equilibrium state. For systems which are time-translation independent, the energy is a conserved quantity, so the average energy is the initial energy—thus we cannot hope for measurements to be independent of the initial energy. Therefore, for each energy E we look at the constant energy surface, Ω_E, in phase space, and for each $w \in \Omega_E$ and each continuous function f on Ω_E we hope that

$$\lim_{T\to\infty} (1/T) \int_0^T f(T_t w)\, dt$$

exists and is a number, $\mu(f)$, independent of w. The map $f \mapsto \mu(f)$ clearly has three properties:

(a) $\mu(1) = 1$
(b) μ is linear.
(c) $\mu(f) \geq 0$ if $f \geq 0$.

We will eventually see (Section IV.4) that such a μ is always associated with a measure $\hat{\mu}$ on Ω_E with $\hat{\mu}(\Omega_E) = 1$, so that

$$\mu(f) = \int_{\Omega_E} f(w)\, d\hat{\mu}(w)$$

Notice that if $f \in L^2(M_1, d\mu_1)$, $g \in L^2(M_2, d\mu_2)$, then

$$\begin{aligned} U(f \otimes g) &= U\Big(\sum c_k \varphi_k \otimes \sum d_\ell \psi_\ell\Big) \\ &= U\Big(\sum_{k,\ell} c_k d_\ell \varphi_k \otimes \psi_\ell\Big) \\ &= \sum_{k,\ell} c_k d_\ell \varphi_k(x)\psi_\ell(y) \\ &= f(x)g(y) \end{aligned}$$

Because of this property, we often say that $L^2(M_1 \times M_2, d\mu_1 \otimes d\mu_2)$ and $L^2(M_1, d\mu_1) \otimes L^2(M_2, d\mu_2)$ are "naturally" isomorphic. Let $M_i = \mathbb{R}$ and $\mu_i =$ Lebesgue measure, then we have shown that $L^2(\mathbb{R}^2)$ is naturally isomorphic to $L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$.

Let us return for a moment to Example 6 of Section II.1: $\langle M, \mu\rangle$ is a measure space and $\mathscr{H}'$ a separable Hilbert space with basis $\{\varphi_k\}$. In Problem 12, the reader is asked to show that each $g \in L^2(M, d\mu; \mathscr{H}')$ is a limit

$$g(x) = \lim_{N\to\infty} \sum_{k=1}^{N} (\varphi_k, g(x))_{\mathscr{H}'} \varphi_k$$

of finite linear combinations of vectors of the form $f_k(x)\varphi_k$, $f_k(x) \in L^2(M, d\mu)$. We now define

$$U: \sum_{k=1}^{N} f_k(x) \otimes \varphi_k \to \sum_{k=1}^{N} f_k(x)\varphi_k$$

Then U is a well-defined map from a dense set in $L^2(M, d\mu) \otimes \mathscr{H}'$ onto a dense set in $L^2(M, d\mu; \mathscr{H}')$ which preserves norms, so U extends uniquely to a unitary operator from $L^2(M, d\mu) \otimes \mathscr{H}'$ to $L^2(M, d\mu; \mathscr{H}')$. Notice that under this map, $U(f(x) \otimes \varphi) = f(x)\varphi$ for all $\varphi \in \mathscr{H}'$. In this sense, U is called the natural isomorphism between $L^2(M, d\mu) \otimes \mathscr{H}'$ and $L^2(M, d\mu; \mathscr{H}')$. We summarize this discussion in a theorem:

Theorem II.10 Let $\langle M_1, \mu_1\rangle$ and $\langle M_2, \mu_2\rangle$ be measure spaces so that $L^2(M_1, d\mu_1)$ and $L^2(M_2, d\mu_2)$ are separable. Then

(a) There is a unique isomorphism from $L^2(M_1, d\mu_1) \otimes L^2(M_2, d\mu_2)$ to $L^2(M_1 \times M_2, d\mu_1 \otimes d\mu_2)$ so that $f \otimes g \mapsto fg$.

(b) If $\mathscr{H}'$ is a separable Hilbert space, then there is a unique isomorphism from $L^2(M_1, d\mu_1) \otimes \mathscr{H}'$ to $L^2(M_1, d\mu_1; \mathscr{H}')$ so that $f(x) \otimes \varphi \mapsto f(x)\varphi$.

(c) There is a unique isomorphism from $L^2(M_1 \times M_2, d\mu_1 \otimes d\mu_2)$ to $L^2(M_1, d\mu_1; L^2(M_2, d\mu_2))$ such that $f(x, y)$ is taken into the function $x \mapsto f(x, \cdot)$.

Example 1 The Hilbert space in the quantum-mechanical description of a single Schrödinger particle of spin one-half is $L^2(\mathbb{R}^3, dx; \mathbb{C}^2)$, that is, the set of pairs $\{\psi_1(x), \psi_2(x)\}$ of square-integrable functions (dx is Lebesgue measure). By what we have shown above, $L^2(\mathbb{R}^3, dx; \mathbb{C}^2)$ is naturally isomorphic to $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$.

Example 2 (Fock spaces) Let $\mathscr{H}$ be a Hilbert space and denote by $\mathscr{H}^n$ the n-fold tensor product $\mathscr{H}^n = \mathscr{H} \otimes \mathscr{H} \otimes \cdots \otimes \mathscr{H}$. Set $\mathscr{H}^0 = \mathbb{C}$ and define

$$\mathscr{F}(\mathscr{H}) = \bigoplus_{n=0}^{\infty} \mathscr{H}^n$$

$\mathscr{F}(\mathscr{H})$ is called the Fock space over $\mathscr{H}$; it will be separable if $\mathscr{H}$ is. For example, if $\mathscr{H} = L^2(\mathbb{R})$, then an element $\psi \in \mathscr{F}(\mathscr{H})$ is a sequence of functions

$$\psi = \{\psi_0, \psi_1(x_1), \psi_2(x_1, x_2), \psi_2(x_1, x_2, x_3), \ldots\}$$

so that

$$|\psi_0|^2 + \sum_{n=1}^{\infty} \int_{\mathbb{R}^n} |\psi_n(x_1, \ldots, x_n)|^2 \, dx_1 \cdots dx_n < \infty$$

Actually, it is not $\mathscr{F}(\mathscr{H})$ itself, but two of its subspaces which are used most frequently in quantum field theory. These two subspaces are constructed as follows: Let $\mathscr{P}_n$ be the permutation group on n elements and let $\{\varphi_k\}$ be a basis for $\mathscr{H}$. For each $\sigma \in \mathscr{P}_n$, we define an operator (which we also denote by σ) on basis elements of $\mathscr{H}^{(n)}$ by

$$\sigma(\varphi_{k_1} \otimes \varphi_{k_2} \otimes \cdots \otimes \varphi_{k_n}) = \varphi_{k_{\sigma(1)}} \otimes \varphi_{k_{\sigma(2)}} \cdots \otimes \varphi_{k_{n(p)}}$$

σ extends by linearity to a bounded operator (of norm one) on $\mathscr{H}^n$ so we can define $S_n = (1/n!) \sum_{\sigma \in \mathscr{P}_n} \sigma$. It is an easy exercise (Problem 23) to show that $S_n^2 = S_n$ and $S_n^* = S_n$, so S_n is an orthogonal projection (the reader unfamiliar with adjoints and orthogonal projections should look up their definitions and elementary properties in Chapter VI). The range of S_n is called the n-fold symmetric tensor product of $\mathscr{H}$. In the case where $\mathscr{H} = L^2(\mathbb{R})$ and $\mathscr{H}^n = L^2(\mathbb{R}) \otimes \cdots \otimes L^2(\mathbb{R}) = L^2(\mathbb{R}^n)$, $S_n \mathscr{H}^n$ is just the subspace of $L^2(\mathbb{R}^n)$ of all functions left invariant under any permutation of the variables. We now define

$$\mathscr{F}_s(\mathscr{H}) = \bigoplus_{n=0}^{\infty} S_n \mathscr{H}^n$$

$\mathscr{F}_s(\mathscr{H})$ is called the **symmetric Fock space over** $\mathscr{H}$ or the **Boson Fock space over** $\mathscr{H}$.

From now on we denote the linear functional μ and the measure $\hat{\mu}$, by the same letter μ.

To summarize: We have shown that if

$$\lim_{T\to\infty} (1/T)\int_0^T f(T_t w)\,dt$$

exists for each fixed w and is independent of $w \in \Omega_E$, then there is a measure μ on Ω_E so that

$$\lim_{T\to\infty} (1/T)\int_0^T f(T_t w)\,dt = \int_{\Omega_E} f(w)\,d\mu(w) \tag{II.3}$$

The measure μ has a very important property. Let s be fixed and suppose χ_F is the characteristic function of a measurable set $F \subset \Omega_E$. Then

$$(1/T)\int_0^T \chi_{T_s^{-1}F}(T_t w)\,dt = (1/T)\int_0^T \chi_F(T_s T_t w)\,dt$$

so if the $\lim_{T\to\infty}$ exists, then $\mu(T_s^{-1}F) = \mu(F)$, that is, the measure is **invariant**. We also say that T is **measure preserving**. Classical mechanical systems come equipped with a natural invariant measure: if $\Gamma = \mathbb{R}^{6N}$ (N is the number of particles), the measure $d^{3N}q\,d^{3N}p$ is known to be invariant under the Hamiltonian flow (Liouville's theorem). This measure has a restriction to Ω_E given formally by

$$\mu_E(F) = \int_F \delta(H(p,q) - E)\,d^{3N}p\,d^{3N}q$$

where $H(p,q)$ is the Hamiltonian. Explicitly, if we pick a set of local coordinates at $x \in \Omega_E$, say $Q_1, \ldots, Q_{6N-1}$, which are orthogonal and normalized, then

$$d\mu_E = C\,d^{6N-1}Q/|\text{grad } H|$$

C is picked so that $\mu_E(\Omega_E) = 1$. Thus, the goal in justifying the zeroth law is to consider

$$M_T(f)(w) = (1/T)\int_0^T f(T_t w)\,dt$$

and to prove that in a suitable sense the function $(M_T f)(w)$ converges as $T \to \infty$ to the constant function with value

$$\int_{\Omega_E} f(w)\,d\mu_E(w)$$

Notice that if we can prove this, we will have proven much more; not only will we have shown that measurements over long periods of time are independent

of the initial conditions (except for the energy), but we will have shown that the equilibrium state is described by a measure in phase space and this measure is

$$\int_F \delta(H(p,q) - E)\, d^{3N}p\, d^{3N}q$$

the "microcanonical ensemble."

Hilbert space methods are so powerful that as soon as one has a measure, it is tempting to try to reformulate the problem in terms of $L^2(\Omega_E, d\mu_E)$. Therefore, if $f \in L^2(\Omega_E, \mu_E)$, we define a map $f \xrightarrow{U_t} f \circ T_t$, that is,

$$(U_t f)(w) = f(T_t w)$$

Lemma (Koopman's lemma) U_t is a unitary map of $L^2(\Omega_E, d\mu_E)$ onto $L^2(\Omega_E, d\mu_E)$.

Proof
$$(U_t f, U_t g) = \int_{\Omega_E} \overline{f(T_t w)} g(T_t w)\, d\mu_E(w)$$
$$= \int_{\Omega_E} \overline{f(y)} g(y)\, d\mu_E(T_t^{-1} y) = \int_{\Omega_E} \overline{f(y)} g(y)\, d\mu_E(y)$$
$$= (f, g)$$

where we have used the invariance of the measure μ_E. Since $U_t U_{-t} = U_0 = I$, U is invertible and thus unitary. ∎

We want to study

$$\frac{1}{T}\int_0^T (U_t f)(w)\, d\mu(w)$$

but it is simpler to consider the discrete analogue

$$\frac{1}{N}\sum_{m=0}^{N-1} U^m f$$

The following elegant result settles the convergence question in the discrete case. Problem 18 extends the discrete result to the continuous case.

Theorem II.11 (mean ergodic theorem, or von Neumann's ergodic theorem) Let U be a unitary operator on a Hilbert space $\mathscr{H}$. Let P be the orthogonal projection onto $\{\psi \mid \psi \in \mathscr{H}, U\psi = \psi\}$. Then, for any $f \in \mathscr{H}$,

$$\lim_{N\to\infty} \frac{1}{N}\sum_{n=0}^{N-1} U^n f = Pf$$

We first prove an elementary technical lemma:

Lemma (a) If U is unitary, $Uf = f$ if and only if $U^*f = f$.
(b) For any operator on a Hilbert space $\mathscr{H}$, $(\text{Ran } A)^\perp = \text{Ker } A^*$.

Proof To prove (a), notice that both conditions are equivalent to $f = U^{-1}f$.
To prove (b), observe that $\psi \in \text{Ker } A^*$ means that $(\varphi, A^*\psi) = 0$ for all φ in $\mathscr{H}$. But, $\psi \in (\text{Ran } A)^\perp$ means that $(A\varphi, \psi) = 0$ for all $\varphi \in \mathscr{H}$. (b) now follows from the definition of adjoint. ∎

Proof of the mean ergodic theorem First let $f = g - Ug$, that is, $f \in \text{Ran}(I - U)$. Then,

$$\left\| \frac{1}{N} \sum_{n=0}^{N-1} U^n f \right\| = \left\| \frac{1}{N} (g - U^N g) \right\| \leq \frac{2\|g\|}{N} \to 0$$

as $N \to \infty$. By an $\varepsilon/3$ argument

$$\frac{1}{N} \sum_{n=0}^{N-1} U^n f \to 0$$

for any $f \in \overline{\text{Ran}(I - U)}$. By the lemma, $(\text{Ran}(I - U))^\perp = \text{Ker}(I - U^*) = \{\psi \mid U^*\psi = \psi\} = \{\psi \mid U\psi = \psi\}$. Therefore, $Pf = 0$ if and only if $f \in \overline{\text{Ran}(I - U)}$. Now, suppose $Pf = f$. Trivially,

$$\frac{1}{N} \sum_{n=0}^{N-1} U^n f = f$$

converges to $f = Pf$. Thus the limit statement holds on $\overline{\text{Ran}(I - U)}$ and on $\text{Ker}(I - U^*)$ and therefore on $\overline{\text{Ran}(I - U)} \oplus \text{Ker}(I - U^*)$, which is all of $\mathscr{H}$ by the projection theorem and (b) above. ∎

In the continuous case $U_t f = f \circ T_t$, what are the functions in $L^2(\Omega_E, d\mu_E)$ which satisfy $U_t f = f$? Clearly, the constant functions are invariant.

Definition T_t is called **ergodic** if the constant functions are the only functions in $L^2(\Omega_E, d\mu_E)$ for which $f \circ T_t = f$ (as L^2 functions) for all t.

Given the continuous analogue of the mean ergodic theorem (Problem 18) we have:

Corollary Let T_t be ergodic. Then for any $f \in L^2(\Omega_E, d\mu_E)$,

$$L^2 - \lim_{T \to \infty} \frac{1}{T} \int_0^T f(T_t w)\, dt = \int_{\Omega_E} f(y)\, d\mu_E(y) \tag{II.4}$$

Proof In this case $\{\psi \mid U\psi = \psi\}$ is one dimensional. Thus $P\psi$ is a constant C and

$$C = (1, \psi) = \int_{\Omega_E} \psi(w)\, d\mu_E(w) \quad \blacksquare$$

Notice that if (II.4) holds then $P\psi$ is constant so that T_t must be ergodic; thus ergodicity is necessary and sufficient for (II.4) to hold.

It is sometimes useful to express ergodicity in terms of the measure.

Proposition T_t is ergodic if and only if for all measurable sets $F \subset \Omega_E$, $T_t^{-1}F = F$ for all t implies $\mu_E(F) = 0$ or $\mu_E(F) = 1$.

Proof Suppose T_t is ergodic and $T_t^{-1}F = F$ for all t. Then $f = \chi_F$ is an invariant function so χ_F is constant a.e., which implies $\mu(F) = 0$ or $\mu(F) = 1$.

Conversely, suppose that the second condition holds. Then $\{w \mid f(w) < a\}$ is invariant under T_t so $f(w) < a$ a.e. or $f(w) \geq a$ a.e. Since this is true for all a, $f(w)$ is constant a.e. $\blacksquare$

The condition that $T_t^{-1}F = F$ implies $\mu_E(F) = 0$ or $\mu_E(F) = 1$ is sometimes called **metric transitivity**.

Let us take stock of what we have proven. We have derived a necessary and sufficient condition on the flow T_t so that

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T f(T_t w)\, dt$$

is precisely what we want it to be, but not in the sense of convergence for each w; instead, we have L^2 convergence of $(1/T)\int_0^T f(T_t w)\, dt$ to the constant function

$$\int_{\Omega_E} f(w)\, d\mu(w)$$

This is not surprising since pointwise convergence is not an L^2 notion. By using Hilbert space methods we have given up the chance of proving that

$$\frac{1}{T} \int_0^T f(T_t w)\, dt$$

converges pointwise for each w as $T \to \infty$. Actually, the pointwise limit does exist but this must be proven by entirely different methods. We state the result:

Theorem II.12 (individual or Birkhoff ergodic theorem) Let T be a measure preserving transformation on a measure space $\langle \Omega, \mu \rangle$. Then for any $f \in L^1(\Omega, \mu)$,

$$\lim_{N \to 0} \frac{1}{N} \sum_{n=0}^{N-1} f(T^n x)$$

exists pointwise a.e. and is some function $f^* \in L^1(\Omega, d\mu)$ satisfying $f^*(Tx) = f^*(x)$. If $\mu(\Omega) < \infty$, then

$$\int_\Omega f^*(x)\, d\mu(x) = \int_\Omega f(x)\, d\mu(x)$$

Furthermore, if μ is ergodic and $\mu(\Omega) = 1$, then

$$\frac{1}{N} \sum_{n=0}^{N-1} f(T^n x) \xrightarrow[N \to \infty]{} \int_\Omega f(y)\, d\mu(y)$$

for almost all x.

This theorem is closer to what one wants to justify statistical mechanics than the von Neumann theorem, and it is fashionable to say that the von Neumann theorem is unsuitable for statistical mechanics. We feel that this is an exaggeration. If we had only the von Neumann theorem we could probably live with it quite well. Typically, initial conditions are not precisely measurable anyway, so that one could well associate initial states with measures $f\, d\mu$ where $\int f\, d\mu = 1$, in which case the von Neumann theorem suffices. However, the Birkhoff theorem does hold and is clearly a result that we are happier to use in justifying the statement that phase-space averages and time averages are equal.

Finally, one should ask whether classical mechanical flows on constant energy surfaces are in fact ergodic. Little is known about this interesting but difficult question. However, Sinai has shown recently that a gas of hard spheres in a box is an ergodic system.

NOTES

Section II.1 A good reference for material on Hilbert spaces is the first chapter of the book, *Introduction to Hilbert Space* by Paul Halmos, Chelsea, Bronx, New York, 1957. His book, *A Hilbert Space Problem Book*, Van Nostrand–Reinhold, Princeton, New Jersey, 1967, which consists of problems, hints, and solutions, is very advanced but is a useful learning device as the reader becomes more sophisticated. The standard reference, *Functional*

Analysis, Ungar, New York, 1955 by F. Riesz and B. Sz.-Nagy has applications to integral equations.

Section II.2 The Riesz Lemma was proved independently by F. Riesz, "Sur une espèce de géométrie analytiques des systèms de fonctions summable," *C. R. Acad. Sci. Paris*, **144** (1907), 1409–1411, and by M. Fréchet in "Sur les ensembles de fonctions et les opérations linéaires," *C. R. Acad. Sci. Paris*, **144** (1907), 1414–1416. The Riesz lemma can be used to give a short proof of the existence of adjoint operators in the case of Hilbert spaces. The general definition of adjoint for Banach spaces is given in Chapter VI.

Section II.3 It may seem at first a little strange that $L^2[0, 1]$ is separable since the functions take values at uncountably many points. However, these values cannot be assigned arbitrarily since the function must be measurable, a strong restriction, and furthermore we have identified functions which differ only on a set of measure zero.

The following question often puzzles students of functional analysis. If all infinite-dimensional separable Hilbert spaces are the same (that is, isomorphic to ℓ_2) why do we talk about them? That is, why worry separately about $L^2(\mathbb{R}^n, d\mu)$ if, as a Hilbert space, it is isomorphic to ℓ_2. The answer is that we are often interested not just in the space but in some other structures, for example some bounded operators on the space. It is true that under the isomorphism these operators go over into bounded operators on ℓ_2, but their structure may be easy to analyze on $L^2(\mathbb{R}, d\mu)$ while it is difficult analyze on ℓ_2. This is one of the general features of functional analysis: One tries to choose a representation of the structures with which one is dealing so that the structures are easy to analyze. As a very simple example the reader should think of the principal axis theorem (spectral theorem) for $\mathbb{C}^n$ which says that given a self-adjoint transformation, one can choose an orthonormal basis in $\mathbb{C}^n$ so that the matrix of the transformation in that basis is diagonal. That is, if one chooses the right isomorphic copy of $\mathbb{C}^n$ (change of basis) then the operator becomes especially simple. As the reader will see, this example is the first note of a rather long symphony.

The first proof of the convergence of Fourier series for a large class of functions was given by Dirichlet in 1829. A good reference for both the classical theory and the modern approach is *An Introduction to Harmonic Analysis*, Wiley, New York, 1968, by Y. Katznelson. Recently Carleson has proven the spectacular result that the Fourier series of a function in $L^2[0, 2\pi]$ converges pointwise a.e. in "On the Convergence and Growth of Partial Sums of Fourier Series," *Acta Math.* **116** (1966), 135–157, and R. Hunt has extended this result to various L^p spaces in "On the Convergence of Fourier Series" appearing in *Orthogonal Expansions and their Continuous Analogues* (D. Haimo, ed.), pp. 235–237, Southern Illinois Univ. Press, 1968.

Section II.4 A description of finite tensor products of Hilbert spaces was first given by J. von Neumann and F. Murray in "On Rings of Operators," *Ann. Math.* (2) 37, (1936), 116–229, though tensor products of finite-dimensional spaces were known long before that. For a modern treatment of tensor products, see F. Trèves, *Topological Vector Spaces, Distributions and Kernels*, Academic Press, New York, 1967, or R. Schatten, *A Theory of Cross Spaces*, Princeton University Press, Princeton, N.J., 1950.

The definition and use of the spaces we have called Fock spaces goes back to the original paper by V. Fock: "Konfigurationsraum und Zweite Quantelung," *Z. Phys.* **75** (1932), 622–647. In Chapter X a Fock space is used in the construction of the free field, a field theory satisfying the Wightman axioms.

Section II.5 For a discussion of thermodynamics from a nonstatistical point of view, that is, as a basically empirical subject, see A. B. Pippard, *The Elements of Classical Thermodynamics*, Cambridge Univ. Press, London and New York, 1957.

For a discussion of points of view regarding the zeroth law of thermodynamics which do not embrace the ergodic theorem, see L. P. Landau and E. M. Lifshitz, *Statistical Physics*, Chapter 1, Pergamon, Oxford, 1958, or F. Strocchi: "Microscopic and Macroscopic Quantities in Statistical Mechanics," *Il Nuovo Cimento*, **65B** (1970), 239–265.

For a proof of Liouville's theorem, see M. Goldstein, *Classical Mechanics*, pp. 266–268, Addison-Wesley, Reading, Massachusetts, 1950, or R. Abraham, *Foundations of Mechanics*, p. 108, Benjamin, New York, 1967.

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The von Neumann ergodic theorem was first proven in J. von Neumann, "Proof of the Quasiergodic Hypothesis," *Proc. Nat. Acad. Sci.* (*U.S.A.*) **18** (1932) 70–82. Our proof is due to F. Riesz, "Sur la théorie ergodique," *Comm. Math. Helv.* **17** (1945), 221–239.

The Birkhoff ergodic theorem was proven by G. D. Birkhoff, "Proof of the Ergodic Theorem," *Proc. Nat. Acad. Sci.* (*U.S.A.*) **17** (1931), 656–660. F. Riesz (op. cit.) provided an alternate and simple proof based on the "maximal ergodic theorem" of N. Wiener, "The Ergodic Theorem," *Duke Math. J.* **5** (1939), 1–18, and of K. Yoshida and S. Kakutani, "Birkhoff's Ergodic Theorem and the Maximal Ergodic Theorem," *Proc. Imp. Acad. Tokyo* **15** (1939), 165–168. A further simplification in the proof of the maximal ergodic theorem may be found in A. M. Garsia, "A Simple Proof of E. Hopf's Maximal Ergodic Theorem," *J. Math. Mech.* **14** (1965), 381–382.

For a delightful discussion of the mathematics of ergodic theory, see P. R. Halmos, *Lectures in Ergodic Theory*, Chelsea, Bronx, New York, 1956, and for a historical summary of the subject see P. R. Halmos, "Measurable Transformations," *Bull. Amer. Math. Soc.* **55**, (1948), 1015–1034.

For a discussion of the mean ergodic theorem in a Banach space setting (which includes L^p-mean ergodic theorems for $1 < p < \infty$), see E. Lorch, *Spectral Theory*, pp. 54–56, Oxford Univ. Press, London and New York, 1962.

There are deep connections between notions from information theory and ergodic theory: for a pleasant, readable treatment, see P. Billingsley, *Ergodic Theory and Information*, Wiley, New York, 1965.

Sinai's result on the ergodicity of a hard sphere gas was announced in Ya. Sinai, "On the Foundations of the Ergodic Hypothesis for a Dynamical System of Statistical Mechanics," *Dokl. Akad. Nauk.* **153** (1963) [*Sov. Math. Dokl.* **4**, (1963), 1818–1822]. A sketch of the proof appears in Ya. Sinai, "Ergodicity of Boltzmann's Gas Model" in *Statistical Mechanics, Foundations and Applications* (T. Bak, ed.), Benjamin, New York, 1967. His proof uses important ideas of Krylov, Kolmogorov, and Anosov.

An alternative property to ergodicity which has some of its consequences is proposed in R. Prosser, "Spectral Analysis of Classical Central Force Motion," *J. Math. Phys.* **10** (1969), 2233–2239. Ideal gases with no collisions are shown to have this property.

For many purposes, one wants thermodynamical systems to possess a stronger property than ergodicity known as mixing; this stronger notion expresses the "irreversibility" of thermodynamic systems and it is this stronger notion that Sinai proves. We return to mixing briefly in Chapter VII. For a discussion of the hierarchy of notions related to ergodicity, see V. I. Arnold and A. Avez, *Ergodic Problems of Classical Mechanics*, Benjamin, New York, 1968 and A. S. Wightman, "Statistical Mechanics and Ergodic Theory: An Expository

Lecture," in *Statistical Mechanics at the Turn of the Decade*, (E. Cohen, ed.), Ungar, New York, 1970.

We have been slightly cavalier in our statement that the question of how big T must be for

$$T^{-1}\int_0^T f(w_t)\,dt$$

to be close to its limit is a detailed dynamical question. In a general ergodic system the time necessary for the limit to be reached should be a typical "recurrence time," that is, the typical time needed for the system to return close to its initial state. Usually, in macroscopic systems this time is astronomically long. Thus, an important question to ask is what properties mechanical systems have that make the "relaxation time"; that is, the time to approach equilibrium, so much smaller than the recurrence time. While this is certainly a detailed dynamical question, it suggests there is an additional mechanism at work which one would like to understand.

PROBLEMS

†1. (a) Let V be an inner product space. Prove that the inner product can be extended to $\tilde{V}$ as follows: First, show that if $x, y \in \tilde{V}$, $x_n, y_n \in V$ and $x_n \to x$, $y_n \to y$, then (x_n, y_n) converges. Define $(x, y) = \lim_{n\to\infty}(x_n, y_n)$ and show that it is independent of which convergent sequences are chosen. Finally, show that $(\cdot, \cdot)$ has the right properties.

(b) Prove the statement in (a) by applying the B.L.T. theorem twice.

*2. (a) A simple function is a finite linear combination of the characteristic functions of disjoint measurable sets. Show that the simple functions are dense in $L^2[a, b]$.

(b) Show that any simple function on $[a, b]$ can be approximated arbitrarily closely (in the L^2 sense) by a step function.

(c) Show that any step function can be approximated arbitrarily closely (in the L^2 sense) by a continuous function and thus conclude that $C[a, b]$ is dense in $L^2[a, b]$ in the L^2 norm.

3. Prove that if μ_1 and μ_2 are mutually singular Borel measures on $\mathbb{R}$ and $\mu = \mu_1 + \mu_2$, then $L^2(\mathbb{R}, d\mu)$ is naturally isomorphic to $L^2(\mathbb{R}, d\mu_1) \oplus L^2(\mathbb{R}, d\mu_2)$. (Hint: let A be a set with $\mu_1(A) = 0$ and $\mu_2(\mathbb{R}\backslash A) = 0$ and map f to $\langle (1 - \chi_A)f, \chi_A f\rangle$.)

4. (a) Prove that the inner product can be recovered from the norm by the **polarization identity**

$$(x, y) = \tfrac{1}{4}\{(\|x + y\|^2 - \|x - y\|^2) - i(\|x + iy\|^2 - \|x - iy\|^2)\}$$

*(b) Prove that a normed linear space is an inner product space if and only if the norm satisfies the parallelogram law.

5. Let V be an inner product space and let $\{x_n\}_{n=1}^N$ be an orthonormal set. Prove that

$$\left\| x - \sum_{n=1}^{N} c_n x_n \right\|$$

is minimized by choosing $c_n = (x_n, x)$.

†6. Let $\mathscr{M}$ be any linear subset of a Hilbert space $\mathscr{H}$. Prove that $\mathscr{M}^\perp$ is a closed linear subspace and that $\bar{\mathscr{M}} = (\mathscr{M}^\perp)^\perp$.

†7. Prove the uniqueness statements in Theorem II.3 and the preceding lemma.

†8. Complete the proof of the corollary to the Riesz Lemma.

9. Let $\mathscr{M}$ be a subspace of a Hilbert space $\mathscr{H}$. Let $f: \mathscr{M} \to \mathbb{C}$ be a linear functional on $\mathscr{M}$ with bound C. Prove that there is a unique extension of f to a continuous linear functional on $\mathscr{H}$ with the same bound. (We note that the existence part of this statement is just the Hahn–Banach theorem for Hilbert spaces, see Section III.3.)

10. Apply the Gram–Schmidt process to the functions $1, x, x^2, x^3$ on the interval $[-1, 1]$ with the L^2 inner product and obtain the first four Legendre polynomials (up to constant multiples).

11. Prove that $L^2(\mathbb{R})$ is separable. (Hint: see Problem 2.)

†12. (Example 6, Section II.1) We say that a vector-valued function f from a measure space $\langle X, \mu\rangle$ to a separable Hilbert space, $\mathscr{H}'$, is measurable if $(y, f(x))_{\mathscr{H}'}$ is measurable for each $y \in \mathscr{H}'$.

(a) Show that if $f(x)$ and $g(x)$ are measurable vector-valued functions, then $\|f(x)\|^2_{\mathscr{H}'}$ and $(f(x), g(x))_{\mathscr{H}'}$ are measurable.

(b) Let $\{\varphi_k\}_{k=1}^\infty$ be a basis for $\mathscr{H}'$. Prove that if $g \in L^2(X, d\mu; \mathscr{H}')$, then

$$\sum_{k=1}^{N} (\varphi_k, g(x))_{\mathscr{H}'} \varphi_k \to g$$

and if $f \in L^2(X, d\mu; \mathscr{H}')$

$$(f, g) = \sum_{k=1}^{\infty} \int_X (f(x), \varphi_k)_{\mathscr{H}'} (\varphi_k, g(x))_{\mathscr{H}'} \, d\mu(x)$$

(c) Assume that $L^2(X, d\mu)$ is separable and prove that $L^2(X, d\mu; \mathscr{H}')$ is separable.

13. Using direct sums, construct an inseparable Hilbert space and an uncountable orthonormal basis.

*14. The goal of this exercise is to prove that the Fourier series of a continuous function is pointwise Césaro summable to f. View $[0, 2\pi]$ as a group with addition mod 2π and write $\int_0^{2\pi}$ as $\oint$. Let $f(\theta) \in L^2[0, 2\pi]$ and $c_n = (e^{in\theta}/\sqrt{2\pi}, f)$.

(a) Let $S_N(f) = \sum_{-N}^{N} c_n e^{in\theta}/\sqrt{2\pi}$. Prove that

$$(S_N f)(\theta) = \frac{1}{2\pi} \oint f(\theta + x) \frac{\sin(N + 1/2)x}{\sin(x/2)} \, dx$$

(b) Let $(\sum_n(f))(\theta) = [1/(N+1)] \sum_0^N S_n(f)(\theta)$ (Césaro sum). Prove that

$$\left(\sum_N (f)\right)(\theta) = \frac{1}{2\pi(N+1)} \oint f(x + \theta) \frac{\sin^2[(N+1)/2]x}{\sin^2(x/2)} \, dx$$

(c) Let

$$K_N(x) = \frac{\sin^2[(N+1)/2]x}{2\pi(N+1)\sin^2(x/2)}$$

Prove that for any $\delta > 0$, $K_N(x) \to 0$ uniformly in $[\delta, 2\pi - \delta]$.

(d) Prove that $(\sum_N(f))(\theta_0) \to f(\theta_0)$ if f is bounded and continuous at θ_0.

(e) Prove that if f is continuous and periodic, then $(\sum_N(f))(\theta) \to f(\theta)$ uniformly in θ. (Hint: Recall that f continuous on $[0, 2\pi]$ implies that f is uniformly continuous.)

(f) Show that $\|f - S_N(f)\|_2 \leq \|f - \sum_n(f)\|_2$ and conclude that $S_N(f) \xrightarrow{L_2} f$ if f is continuous.

†*15.* Suppose $f \in C_p^1[0, 2\pi]$ and let $c_n = (e^{inx}/\sqrt{2\pi}, f)$, $b_n = (e^{inx}/\sqrt{2\pi}, f'(x))$.

(a) Prove $\sum |b_n|^2 < \infty$ and conclude that $\sum n^2 |c_n|^2 < \infty$.

(b) Prove that $\sum |c_n| < \infty$.

(c) Prove that $\sum_{-M}^{M} c_n e^{inx}/\sqrt{2\pi}$ is uniformly convergent as $M \to \infty$.

(d) Use 14(f) to conclude that $\sum_{-M}^{M} c_n e^{inx}/\sqrt{2\pi}$ is uniformly convergent to f.

16. Show that the unit ball in an infinite dimensional Hilbert space contains infinitely many *disjoint* translates of a ball of radius $\sqrt{2}/4$. Conclude that one cannot have a nontrivial translation invariant measure on an infinite dimensional Hilbert space.

17. Prove the Poincaré recurrence theorem: Given a measure preserving map, T, on a set Ω with $\mu(\Omega) < \infty$, then for any measurable set $E \subset \Omega$, $T^n x \in E$ infinitely often for almost all $x \in E$. This result says that almost every state returns arbitrarily close to its initial position infinitely often (thus assuring that fluctuations continue to take place). Hint: Let $F = \{x \in E \mid T^n x \notin E \text{ for any } n > 0\}$. Show $\{T^{-m}F\}$ are disjoint and prove thereby that F has measure zero.

18. Let T_t be a one-parameter group of measure-preserving transformations of a measure space $\langle \Omega, \mu \rangle$. Apply the discrete mean ergodic theorem to $\int_0^1 f(T_t w)\, dt$ to prove the mean ergodic theorem for $\lim_{T\to\infty} (1/T) \int_0^T f(T_t w)\, dt$.

19. Let V be an operator in a Hilbert space satisfying $\|V^n\| \leq C$ for all n. Prove that $(1/N)\sum_{n=0}^{N-1} V^n f \to Pf$ for all $f \in \mathscr{H}$ where P is a (not necessarily orthogonal) projection onto $\{f \mid Vf = f\}$.

20. Consider the unit circle, $\{z \in \mathbb{C} \mid |z| = 1\}$ with Lebesgue measure. Let $T(z) = e^{2\pi i\theta} z$. Show that T is ergodic if and only if θ is irrational.

21. Suppose Ω is a compact metric space with metric ρ and some measure μ. Let T be a measure-preserving ergodic transformation with the additional property that $\rho(Tx, Ty) = \rho(x, y)$. (For example, the map T in Problem 20 when θ is irrational.) Show that if f is a continuous function on Ω, then $(1/N)\sum_{n=0}^{N-1} f(T^n w)$ converges *uniformly* to $\int_\Omega f\, d\mu$. (Hint: Prove that the family

$$(M_N f)(w) = \frac{1}{N} \sum_{n=0}^{N-1} f(T^n w)$$

is uniformly equicontinuous and then use the mean ergodic and Ascoli theorems.)

**22.* Let $\{\eta_n\}_{n=-\infty}^{\infty}$ be a set of vectors in a Hilbert space, $\mathscr{H}$, so that $a_{nm} = |(\eta_n, \eta_m)|$ is the matrix (in the natural basis) of an operator A on $\ell_2(-\infty, \infty)$. Prove that

$$\sum_{n=-\infty}^{\infty} |(f, \eta_n)|^2 \leq \|A\|\, \|f\|^2$$

for any $f \in \mathscr{H}$.

23. Let S_n be the operator defined in Example 2 of Section 4.
(a) Prove that S_n is independent of the basis $\{\varphi_k\}$.
(b) Prove that $S_n^2 = S_n$ and $S_n = S_n^*$ (Hint: show that $\sigma^* = \sigma^{-1}$).
(c) Do parts (a) and (b) for A_n.

**24* Let $\langle M, \mathcal{R}, \mu\rangle$ be a σ-finite measure space. Let $\mathcal{R}_F = \{X \in \mathcal{R} \mid \mu(X) < \infty\}$. Call X, $Y \in \mathcal{R}_F$ equivalent if and only if $\mu(X \triangle Y) = 0$ where $X \triangle Y = (X \setminus Y) \cup (Y \setminus X)$. Let $\hat{\mathcal{R}}_F$ be the family of equivalence classes of $\mathcal{R}_F$ under this relation.
(a) Prove that $\mu(X \triangle Y)$ only depends on the equivalence classes of X and Y in $\hat{\mathcal{R}}_F$.
(b) Prove that $\hat{\mathcal{R}}_F$ with the function $\rho(X, Y) = \mu(X \triangle Y)$ is a metric space.
(c) Prove that $L^2(M, d\mu)$ is separable if and only if $\mathcal{R}_F$ with the metric ρ is a separable metric space.

**25.* Find a finite measure space (that is, $\langle M, \mathcal{R}, \mu\rangle$ with $\mu(M) < \infty$) with $L^2(M, d\mu)$ nonseparable. (Hint: Take an uncountable Cartesian product of sets of the form $[0, 1]$.)

26. Prove that part (c) of Theorem II.10 follows from parts (a) and (b).

27. Prove the projection theorem using the existence of orthonormal bases.

III: Banach Spaces

Reductio ad absurdum is one of a mathematician's finest weapons. It is a far finer gambit than any chess gambit: a chess player may offer the sacrifice of a pawn or even a piece, but a mathematician offers the game.

G. H. Hardy

III.1 Definition and examples †

We defined normed linear spaces in Section I.2. Since normed linear spaces are metric spaces, they may have the property of being complete.

Definition A complete normed linear space is called a **Banach space.**

Banach spaces have many of the properties of $\mathbb{R}^n$: they are vector spaces, they have a notion of distance provided by the norm, and every Cauchy sequence has a limit. In general the norm does not arise from an inner product (see Problem 4 of Chapter II), so Banach spaces are not necessarily Hilbert spaces and will not have all of the same nice geometrical properties. In order to acquaint the reader with the types of Banach spaces he is likely to encounter, we discuss several examples in detail.

Example 1 ($L^\infty(\mathbb{R})$ and its subspaces) Let $L^\infty(\mathbb{R})$ be the set of (equivalence classes of) complex-valued measurable functions on $\mathbb{R}$ such that $|f(x)| \leq M$ a.e. with respect to Lebesgue measure for some $M < \infty$ ($f \sim g$ means $f(x) = g(x)$ a.e.). Let $\|f\|_\infty$ be the smallest such M. It is an easy exercise (Problem 1) to

† A supplement to this section begins on p. 348.

show that $L^\infty(\mathbb{R})$ is a Banach space with norm $\|\cdot\|_\infty$. The bounded continuous functions $C(\mathbb{R})$ is a subspace of $L^\infty(\mathbb{R})$ and restricted to $C(\mathbb{R})$ the $\|\cdot\|_\infty$-norm is just the usual supremum norm under which $C(\mathbb{R})$ is complete (since the uniform limit of continuous functions is continuous). Thus, $C(\mathbb{R})$ is a closed subspace of $L^\infty(\mathbb{R})$.

Consider the set $\kappa(\mathbb{R})$ of continuous functions with compact support, that is, the continuous functions that vanish outside of some closed interval. $\kappa(\mathbb{R})$ is a normed linear space under $\|\cdot\|_\infty$ but is not complete. The completion of $\kappa(\mathbb{R})$ is not all of $C(\mathbb{R})$; for example, if f is the function which is identically equal to one, then f cannot be approximated by a function in $\kappa(\mathbb{R})$ since $\|f-g\|_\infty \geq 1$ for all $g \in \kappa(\mathbb{R})$. The completion of $\kappa(\mathbb{R})$ is just $C_\infty(\mathbb{R})$, the continuous functions which approach zero at $\pm\infty$ (Problem 5). Some of the most powerful theorems in functional analysis (Riesz–Markov, Stone–Weierstrass) are generalizations of properties of $C(\mathbb{R})$ (see Sections IV.3 and IV.4).

Example 2 (L^p spaces) Let $\langle X, \mu\rangle$ be a measure space and $p \geq 1$. We denote by $L^p(X, d\mu)$ the set of equivalence classes of measurable functions which satisfy:

$$\|f\|_p \equiv \left(\int_X |f(x)|^p \, d\mu(x)\right)^{1/p} < \infty$$

Two functions are equivalent if they differ only on a set of measure zero. The following theorem collects many of the standard facts about L^p spaces.

Theorem III.1 Let $1 \leq p < \infty$, then

(a) (the Minkowski inequality) If $f, g \in L^p(X, d\mu)$, then

$$\|f+g\|_p \leq \|f\|_p + \|g\|_p$$

(b) (Riesz–Fisher) $L^p(X, d\mu)$ is complete.

(c) (the Hölder inequality) Let p, q, and r be positive numbers satisfying $p, q, r \geq 1$ and $p^{-1} + q^{-1} = r^{-1}$. Suppose $f \in L^p(X, d\mu)$, $g \in L^q(X, d\mu)$. Then $fg \in L^r(X, d\mu)$ and

$$\|fg\|_r \leq \|f\|_p \, \|g\|_q$$

Proofs of many of the basic facts about L^p spaces, including these inequalities, can be found in the second supplemental section. The Minkowski inequality shows that $L^p(X, d\mu)$ is a vector space and that $\|\cdot\|_p$ satisfies the

triangle inequality. Combined with (b) this shows that $L^p(X, d\mu)$ is a Banach space. We have given the proof of (b) for the case where $p = 1$, $X = \mathbb{R}$ and $\mu =$ Lebesgue measure; the proof for the general case is similar.

Example 3 (sequence spaces) There is a nice class of spaces which is easy to describe and which we will often use to illustrate various concepts. In the following definitions,

$$a = \{a_n\}_{n=1}^{\infty}$$

always denotes a sequence of complex numbers.

$$\ell_\infty = \left\{ a \,\middle|\, \|a\|_\infty \equiv \sup_n |a_n| < \infty \right\}$$

$$c_0 = \left\{ a \,\middle|\, \lim_{n\to\infty} a_n = 0 \right\}$$

$$\ell_p = \left\{ a \,\middle|\, |a|_p \equiv \left(\sum_{n=1}^{\infty} |a_n|^p \right)^{1/p} < \infty \right\}$$

$$s = \left\{ a \,\middle|\, \lim_{n\to\infty} n^p a_n = 0 \quad \text{for all positive integers } p \right\}$$

$$f = \left\{ a \,\middle|\, a_n = 0 \quad \text{for all but a finite number of } n \right\}$$

It is clear that as sets $f \subset s \subset \ell_p \subset c_0 \subset \ell_\infty$.

The spaces ℓ_∞ and c_0 are Banach spaces with the $\|\cdot\|_\infty$ norm; ℓ_p is a Banach space with the $\|\cdot\|_p$ norm (note that this follows from Example 2 since $\ell_p = L^p(\mathbb{R}, d\mu)$ where μ is the measure with mass one at each positive integer and zero everywhere else). It will turn out that s is a Fréchet space (Section V.2). One of the reasons that these spaces are easy to handle is that f is dense in ℓ_p (in $\|\cdot\|_p$; $p < \infty$) and is dense in c_0 (in the $\|\cdot\|_\infty$ norm). Actually, the set of elements of f with only rational entries is also dense in ℓ_p and c_0. Since this set is countable, ℓ_p and c_0 are separable. ℓ_∞ is not separable (Problem 2).

Example 4 (the bounded operators) In Section I.3 we defined the concept of a bounded linear transformation or bounded operator from one normed linear space, X, to another Y; we will denote the set of all bounded linear operators from X to Y by $\mathscr{L}(X, Y)$. We can introduce a norm on $\mathscr{L}(X, Y)$ by defining

$$\|A\| = \sup_{x \in X,\, x \neq 0} \frac{\|Ax\|_Y}{\|x\|_X}$$

This norm is often called the **operator norm.**

Theorem III.2 If Y is complete, $\mathscr{L}(X, Y)$ is a Banach space.

Proof Since any finite linear combination of bounded operators is again a bounded operator, $\mathscr{L}(X, Y)$ is a vector space. It is easy to see that $\|\cdot\|$ is a norm; for example, the triangle inequality is proven by the computation

$$\begin{aligned}\|A + B\| &= \sup_{x \neq 0} \frac{\|(A + B)x\|}{\|x\|} \leq \sup_{x \neq 0} \frac{\|Ax\| + \|Bx\|}{\|x\|} \\ &\leq \sup_{x \neq 0} \frac{\|Ax\|}{\|x\|} + \sup_{x \neq 0} \frac{\|Bx\|}{\|x\|} \\ &= \|A\| + \|B\|\end{aligned}$$

To show that $\mathscr{L}(X, Y)$ is complete, we must prove that if $\{A_n\}_{n=1}^{\infty}$ is a Cauchy sequence in the operator norm, then there is a bounded linear operator A so that $\|A_n - A\| \to 0$. Let $\{A_n\}_{n=1}^{\infty}$ be Cauchy in the operator norm; we construct A as follows. For each $x \in X$, $\{A_n x\}_{n=1}^{\infty}$ is a Cauchy sequence in Y. Since Y is complete, $A_n x$ converges to an element $y \in Y$. Define $Ax = y$. It is easy to check that A is a linear operator. From the triangle inequality it follows that

$$|\,\|A_n\| - \|A_m\|\,| \leq \|A_n - A_m\|$$

so $\{\|A_n\|\}_{n=1}^{\infty}$ is a Cauchy sequence of real numbers converging to some real number C. Thus,

$$\begin{aligned}\|Ax\|_Y &= \lim_{n \to \infty} \|A_n x\|_Y \leq \lim_{n \to \infty} \|A_n\|\, \|x\|_X \\ &= C\|x\|_X\end{aligned}$$

so A is a bounded linear operator. We must still show that $A_n \to A$ in the operator norm. Since $\|(A - A_n)x\| = \lim_{m \to \infty} \|(A_m - A_n)x\|$, we have

$$\frac{\|(A - A_n)x\|}{\|x\|} \leq \lim_{n \to \infty} \|A_m - A_n\|$$

which implies

$$\|A - A_n\| = \sup_{x \neq 0} \frac{\|(A - A_n)x\|}{\|x\|} \leq \lim_{m \to \infty} \|A_m - A_n\|$$

which is arbitrarily small for n large enough. The triangle inequality shows that the norm of A is actually equal to C. ∎

It is important to have criteria to determine whether normed linear spaces are complete. Such a criterion is given by the following theorem (whose proof is left to Problem 3). A sequence of elements $\{x_n\}_{n=1}^{\infty}$ in a normed linear

space X is called **absolutely summable** if $\sum_{n=1}^{\infty} \|x_n\| < \infty$. It is called **summable** if $\sum_{n=1}^{N} x_n$ converges as $N \to \infty$ to an $x \in X$.

Theorem III.3 A normed linear space is complete if and only if every absolutely summable sequence is summable.

For a typical application of this theorem, see the construction of quotient spaces in Section III.4. We conclude this introductory section with some definitions.

Definition A bounded linear operator from a normed linear space X to a normed linear space Y is called an **isomorphism** if it is a bijection which is continuous and which has a continuous inverse. If it is norm preserving, it is called an **isometric isomorphism** (any norm preserving map is called an isometry).

For example, we proved in Section II.3 that all separable, infinite-dimensional Hilbert spaces are isometric to ℓ_2. Two Banach spaces which are isometric can be regarded as the same as far as their Banach space properties are concerned.

We will often encounter a situation in which we have two different norms on a normed linear space.

Definition Two norms, $\|\cdot\|_1$ and $\|\cdot\|_2$, on a normed linear space X are called **equivalent** if there are positive constants C and C' such that, for all $x \in X$,

$$C\|x\|_1 \leq \|x\|_2 \leq C'\|x\|_1$$

For example, the following three norms on $\mathbb{R}^2$ are all equivalent:

$$\|\langle x, y\rangle\|_2 = \sqrt{|x|^2 + |y|^2}$$
$$\|\langle x, y\rangle\|_1 = |x| + |y|$$
$$\|\langle x, y\rangle\|_\infty = \max\{|x|, |y|\}$$

In fact, all norms on $\mathbb{R}^2$ are equivalent; see Problem 4. The usual situation we will encounter is an incomplete normed linear space with two norms. The completions of the space in the two norms will be isomorphic if and only if the norms are equivalent. An example is provided by the sequence spaces of Example 3. The completion of f in the $\|\cdot\|_\infty$ norm is c_0 while the completion in the $\|\cdot\|_p$ norm is ℓ_p. Two norms, $\|\cdot\|_1$ and $\|\cdot\|_2$, on a normed linear space X are equivalent if and only if the identity map is an isomorphism from $\langle X, \|\cdot\|_1\rangle$ to $\langle X, \|\cdot\|_2\rangle$.

III.2 Duals and double duals

In the last section we proved that the set of bounded linear transformations from one Banach space X to another Y was itself a Banach space. In the case where Y is the complex numbers, this space $\mathscr{L}(X, \mathbb{C})$ is denoted by X^* and called the **dual space** of X. The elements of X^* are called bounded linear functionals on X. In this chapter when we talk about convergence in X^* we always mean convergence in the norm given in Theorem III.2. If $\lambda \in X^*$, then

$$\|\lambda\| = \sup_{x \in X,\ \|x\| \leq 1} |\lambda(x)|$$

In Section IV.5, we discuss another notion of convergence for X^*.

Dual spaces play an important role in mathematical physics. In many models of physical systems, whether in quantum mechanics, statistical mechanics, or quantum field theory, the possible states of the system in question can be associated with linear functionals on appropriate Banach spaces. Furthermore, linear functionals are important in the modern theory of partial differential equations. For these reasons, and because they are interesting in their own right, dual spaces have been studied extensively. There are two directions in which such study can proceed: either determining the dual spaces of particular Banach spaces or proving general theorems relating properties of Banach spaces to properties of their duals. In this section we study several examples of special interest and prove one general theorem. For an example of another general theorem see Theorem III.7.

Example 1 (L^p spaces) Suppose that $1 < p < \infty$ and $p^{-1} + q^{-1} = 1$. If $f \in L^p(\mathbb{R})$ and $g \in L^q(\mathbb{R})$ then, according to the Hölder inequality (Theorem III.1), fg is in $L^1(\mathbb{R})$. Thus,

$$\int_{-\infty}^{\infty} \overline{g(x)} f(x)\, dx$$

makes sense. Let $g \in L^q(\mathbb{R})$ be fixed and define

$$G(f) = \int_{-\infty}^{\infty} \bar{g} f\, dx$$

for each $f \in L^p(\mathbb{R})$. The Hölder inequality shows that $G(\cdot)$ is a bounded linear functional on $L^p(\mathbb{R})$ with norm less than or equal to $\|g\|_q$; actually the norm is equal to $\|g\|_q$. The converse of this statement is also true. That is, every bounded linear functional on L^p is of the form $G(\cdot)$ for some $g \in L^q$. Furthermore, different functions in L^q give rise to different functionals on L^p. Thus,

the mapping that assigns to each $g \in L^q$ the corresponding linear functional, $G(\cdot)$, on $L^p(\mathbb{R})$ is a (conjugate linear) isometric isomorphism of L^q onto $(L^p)^*$. In this sense, L^q is the dual of L^p. Since the roles of p and q in the expression $p^{-1} + q^{-1} = 1$ are symmetric, it is clear that $L^p = (L^q)^* = ((L^p)^*)^*$. That is, the dual of the dual of L^p is again L^p.

The case where $p = 1$ is different. The dual of $L^1(\mathbb{R})$ is $L^\infty(\mathbb{R})$ with the elements of $L^\infty(\mathbb{R})$ acting on functions in $L^1(\mathbb{R})$ in the natural way given by the above integral. However, the dual of $L^\infty(\mathbb{R})$ is not $L^1(\mathbb{R})$ but a much larger space (see Problems 7 and 8). As a matter of fact, we will prove later (Chapter XVI) that $L^1(\mathbb{R})$ is not the dual of any Banach space. The duality statements in this example hold for $L^p(X, d\mu)$ where $\langle X, \mu \rangle$ is a general measure space except that $L^1(X)$ may be the dual of $L^\infty(X)$ if $\langle X, \mu \rangle$ is trivially small.

Example 2 (Hilbert spaces) If we let $p = 2$ in Example 1, then $q = 2$ and we obtain the result that $L^2(\mathbb{R}) = L^2(\mathbb{R})^*$, that is, $L^2(\mathbb{R})$ is its own dual space. In fact, we have already shown (the Riesz lemma) in Section II.2 that this is true for all Hilbert spaces. The reader is cautioned again that the map which identifies $\mathscr{H}$ with its dual $\mathscr{H}^*$ is conjugate linear. If $g \in \mathscr{H}$, then the linear functional G corresponding to g is $G(f) = (g, f)$.

Example 3 $(\ell_\infty = \ell_1^*, \ell_1 = c_0^*)$ Suppose that $\{\lambda_k\}_{k=1}^\infty \in \ell_1$. Then for each $\{a_k\}_{k=1}^\infty \in c_0$

$$\Lambda(\{a_k\}_{k=1}^\infty) = \sum_{k=1}^\infty \lambda_k a_k$$

converges and $\Lambda(\cdot)$ is a continuous linear functional on c_0 with norm equal to $\sum_{k=1}^\infty |\lambda_k|$. To see that all continuous linear functionals on c_0 arise in this way, we proceed as follows. Suppose $\lambda \in c_0^*$ and let e^k be the sequence in c_0 which has all its terms equal to zero except for a one in the kth place. Define $\lambda_k = \lambda(e^k)$ and let $f^\ell = \sum_{k=1}^\ell (|\lambda_k|/\lambda_k) e^k$. If some λ_k is zero, we simply omit that term from the sum. Then for each ℓ, $f^\ell \in c_0$ and $\|f^\ell\|_{c_0} = 1$. Since,

$$\lambda(f^\ell) = \sum_{k=1}^\ell |\lambda_k| \qquad \text{and} \qquad |\lambda(f^\ell)| \leq \|f^\ell\|_{c_0} \|\lambda\|_{c_0^*}$$

we have

$$\sum_{k=1}^\ell |\lambda_k| \leq \|\lambda\|_{c_0^*}$$

Since this is true for all ℓ, $\sum_{k=1}^\infty |\lambda_k| < \infty$ and

$$\Lambda(\{a_k\}_{k=1}^\infty) = \sum_{k=1}^\infty \lambda_k a_k$$

is a well-defined linear functional on c_0. However, $\lambda(\cdot)$ and $\Lambda(\cdot)$ agree on finite linear combinations of the e_k. Because such finite linear combinations are dense in c_0, we conclude that $\lambda = \Lambda$. Thus every functional in c_0^* arises from a sequence in ℓ_1, and the reader can check for himself that the norms in ℓ_1 and c_0^* coincide. Thus $\ell_1 = c_0^*$. A similar proof shows that $\ell_\infty = \ell_1^*$.

Since the dual X^* of a Banach space is itself a Banach space (Theorem III.2), it also has a dual space, denoted by X^{**}. X^{**} is called the **second dual,** the **bidual,** or the **double dual** of the space X. In Example 3, ℓ_1 is the first dual of c_0 and ℓ_∞ is the second dual. It is not a priori evident that X^* is always nonzero and if $X^* = \{0\}$ then $X^{**} = \{0\}$ too. However, this situation does not occur; dual spaces always have plenty of linear functionals in them. We prove this fact in the next section. Using a corollary also proven there we will prove that X can be regarded in a natural way as a subset of X^{**}.

Theorem III.4 Let X be a Banach space. For each $x \in X$, let $\tilde{x}(\cdot)$ be the linear functional on X^* which assigns to each $\lambda \in X^*$ the number $\lambda(x)$. Then the map $J: x \to \tilde{x}$ is an isometric isomorphism of X onto a (possibly proper) subspace of X^{**}.

Proof Since

$$|\tilde{x}(\lambda)| = |\lambda(x)| \leq \|\lambda\|_{X^*}\|x\|_X$$

$\tilde{x}$ is a bounded linear functional on X^* with norm $\|\tilde{x}\|_{X^{**}} \leq \|x\|_X$. It follows from Theorems III.5 and III.6 that, given x, we can find a $\lambda \in X^*$ so that

$$\|\lambda\|_{X^*} = 1 \qquad \text{and} \qquad \lambda(x) = \|x\|_X$$

This shows that

$$\|\tilde{x}\|_{X^{**}} = \sup_{\lambda \in X^*,\ \|\lambda\| \leq 1} |\tilde{x}(\lambda)| \geq \|x\|_X$$

which implies that

$$\|\tilde{x}\|_{X^{**}} = \|x\|_X$$

Thus, J is an isometry of X into X^{**}. ∎

Definition If the map J, defined in Theorem III.4, is surjective, then X is said to be **reflexive.**

The $L^p(\mathbb{R})$ spaces are reflexive for $1 < p < \infty$ since $(L^p)^{**} = (L^q)^* = L^p$, but $L^1(\mathbb{R})$ is not reflexive. All Hilbert spaces are reflexive. c_0 is not reflexive, since its double dual is ℓ_∞. The theory of reflexive spaces is developed further in Problems 22 and 26 of this chapter and Problem 15 of Chapter V.

III.3 The Hahn–Banach theorem

In dealing with Banach spaces, one often needs to construct linear functionals with certain properties. This is usually done in two steps: first one defines the linear functional on a subspace of the Banach space where it is easy to verify the desired properties; second, one appeals to (or proves) a general theorem which says that any such functional can be extended to the whole space while retaining the desired properties. One of the basic tools of the second step is the following theorem, whose variants will reappear in Section V.1 and Chapter XIV.

Theorem III.5 (Hahn–Banach theorem) Let X be a real vector space, p a real-valued function defined on X satisfying $p(\alpha x + (1-\alpha)y) \le \alpha p(x) + (1-\alpha)p(y)$ for all x and y in X and all $\alpha \in [0, 1]$. Suppose that λ is a linear functional defined on a subspace Y of X which satisfies $\lambda(x) \le p(x)$ for all $x \in Y$. Then, there is a linear functional Λ, defined on X, satisfying $\Lambda(x) \le p(x)$ for all $x \in X$, such that $\Lambda(x) = \lambda(x)$ for all $x \in Y$.

Proof The idea of the proof is the following. First we will show that if $z \in X$ but $z \notin Y$, then we can extend λ to a functional having the right properties on the space spanned by z and Y. We then use a Zorn's lemma argument to show that this process can be continued to extend λ to the whole space X.

Let $\tilde{Y}$ denote the subspace spanned by Y and z. The extension of λ to Y, call it $\tilde{\lambda}$, is specified as soon as we define $\tilde{\lambda}(z)$ since

$$\tilde{\lambda}(az + y) = a\tilde{\lambda}(z) + \lambda(y)$$

Suppose that $y_1, y_2 \in Y$, $\alpha, \beta > 0$. Then

$$\beta\lambda(y_1) + \alpha\lambda(y_2) = \lambda(\beta y_1 + \alpha y_2) = (\alpha+\beta)\lambda\left(\frac{\beta}{\alpha+\beta}\, y_1 + \frac{\alpha}{\alpha+\beta}\, y_2\right)$$

$$\le (\alpha+\beta)p\left(\frac{\beta}{\alpha+\beta}\,(y_1 - \alpha z) + \frac{\alpha}{\alpha+\beta}\,(y_2 + \beta z)\right)$$

$$\le \beta p(y_1 - \alpha z) + \alpha p(y_2 + \beta z)$$

Thus, for all $\alpha, \beta > 0$ and $y_1, y_2 \in Y$,

$$\frac{1}{\alpha}\,[-p(y_1 - \alpha z) + \lambda(y_1)] \le \frac{1}{\beta}\,[p(y_2 + \beta z) - \lambda(y_2)]$$

We can therefore find a real number a such that

$$\sup_{\substack{y\in Y\\ \alpha>0}}\left[\frac{1}{\alpha}(-p(y-\alpha z)+\lambda(y))\right]\le a\le\inf_{\substack{y\in Y\\ \alpha>0}}\left[\frac{1}{\alpha}(p(y+\alpha z)-\lambda(y))\right]$$

We now define $\tilde{\lambda}(z)=a$. It may be easily verified that the resulting extension satisfies $\tilde{\lambda}(x)\le p(x)$ for all $x\in\tilde{Y}$. This shows that λ can be extended one dimension at a time.

We now proceed with the Zorn's lemma argument. Let $\mathscr{E}$ be the collection of extensions e of λ which satisfy $e(x)\le p(x)$ on the subspace where they are defined. We partially order $\mathscr{E}$ by setting $e_1\prec e_2$ if e_2 is defined on a larger set than e_1 and $e_2(x)=e_1(x)$ where they are both defined. Let $\{e_\alpha\}_{\alpha\in A}$ be a linearly ordered subset of $\mathscr{E}$; let X_α be the subspace on which e_α is defined. Define e on $\bigcup_{\alpha\in A}X_\alpha$ by setting $e(x)=e_\alpha(x)$ if $x\in X_\alpha$. Clearly $e_\alpha\prec e$ so each linearly ordered subset of $\mathscr{E}$ has an upper bound. By Zorn's lemma, $\mathscr{E}$ has a maximal element Λ, defined on some set X', satisfying $\Lambda(x)\le p(x)$ for $x\in X'$. But, X' must be all of X, since otherwise we could extend Λ to a $\tilde{\Lambda}$ on a larger space by adding one dimension as above. Since this contradicts the maximality of Λ, we must have $X=X'$. Thus, the extension Λ is everywhere defined. ∎

In the theorem we have just proven, X is a real vector space. We now extend the theorem to the case where X is complex.

Theorem III.6 (complex Hahn–Banach theorem) Let X be a complex vector space, p a real-valued function defined on X satisfying $p(\alpha x+\beta y)\le|\alpha|p(x)+|\beta|p(y)$ for all $x,y\in X$, and $\alpha,\beta\in\mathbb{C}$ with $|\alpha|+|\beta|=1$. Let λ be a complex linear functional defined on a subspace Y of X satisfying $|\lambda(x)|\le p(x)$ for all $x\in Y$. Then, there exists a complex linear functional Λ, defined on X, satisfying $|\Lambda(x)|\le p(x)$ for all $x\in X$ and $\Lambda(x)=\lambda(x)$ for all $x\in Y$.

Proof Let $\ell(x)=\mathrm{Re}\{\lambda(x)\}$. ℓ is a real linear functional on Y and since

$$\ell(ix)=\mathrm{Re}\{\lambda(ix)\}=\mathrm{Re}\{i\lambda(x)\}=-\mathrm{Im}\{\lambda(x)\}$$

we see that $\lambda(x)=\ell(x)-i\ell(ix)$. Since ℓ is real linear and $p(\alpha x+(1-\alpha)y)\le\alpha p(x)+(1-\alpha)p(y)$ for $\alpha\in[0,1]$, ℓ has a real linear extension L to all of X obeying $L(x)\le p(x)$ (by Theorem III.5). Define $\Lambda(x)=L(x)-iL(ix)$. Λ clearly extends λ and is real linear. Moreover, $\Lambda(ix)=L(ix)-iL(-x)=i\Lambda(x)$, so Λ is also complex linear. To complete the proof, we need only show

that $|\Lambda(x)| \leq p(x)$. First, note that $p(\alpha x) = p(x)$ if $|\alpha| = 1$. If we let $\theta = \text{Arg}\{\Lambda(x)\}$ and use the fact that $\text{Re}\,\Lambda = L$, we see that

$$\begin{aligned} |\Lambda(x)| &= e^{-i\theta}\Lambda(x) = \Lambda(e^{-i\theta}x) = L(e^{-i\theta}x) \\ &\leq p(e^{-i\theta}x) = p(x) \quad \blacksquare \end{aligned}$$

Corollary 1 Let X be a normed linear space, Y a subspace of X, and λ an element of Y^*. Then there exists a $\Lambda \in X^*$ extending λ and satisfying $\|\Lambda\|_{X^*} = \|\lambda\|_{Y^*}$.

Proof Choose $p(x) = \|\lambda\|_{Y^*}\|x\|$ and apply the above theorems. ∎

Corollary 2 Let y be an element of a normed linear space X. Then there is a nonzero $\Lambda \in X^*$ such that $\Lambda(y) = \|\Lambda\|_{X^*}\|y\|$.

Proof Let Y be the subspace consisting of all scalar multiples of y and define $\lambda(ay) = a\|y\|$. By using Corollary 1, we can construct Λ with $\|\Lambda\| = \|\lambda\|$ extending λ to all of X. But, since $\Lambda(y) = \|y\|$, $\|\Lambda\| = 1$ and therefore

$$\Lambda(y) = \|\Lambda\|_{X^*}\|y\| \quad \blacksquare$$

Corollary 3 Let Z be a subspace of a normed linear space X and suppose that y is an element of X whose distance from Z is d. Then there exists a $\Lambda \in X^*$ so that $\|\Lambda\| \leq 1$, $\Lambda(y) = d$, and $\Lambda(z) = 0$ for all z in Z.

The proof of the third corollary is left to the reader (Problem 10). To show how useful these corollaries are we prove the following general theorem.

Theorem III.7 Let X be a Banach space. If X^* is separable, then X is separable.

Proof Let $\{\lambda_n\}$ be a dense set in X^*. Choose $x_n \in X$, $\|x_n\| = 1$, so that

$$|\lambda_n(x_n)| \geq \|\lambda_n\|/2$$

Let $\mathcal{D}$ be the set of all finite linear combinations of the $\{x_n\}$ with rational coefficients. Since $\mathcal{D}$ is countable, it is sufficient to show that $\mathcal{D}$ is dense in X. If $\mathcal{D}$ is not dense in X, then there is a $y \in X \backslash \mathcal{D}$ and a linear functional $\lambda \in X^*$ so that $\lambda(y) \neq 0$, but $\lambda(x) = 0$ for all $x \in \mathcal{D}$ (Corollary 3). Let $\{\lambda_{n_k}\}$ be a subsequence of $\{\lambda_n\}$ which converges to λ. Then

$$\begin{aligned} \|\lambda - \lambda_{n_k}\|_{X^*} &\geq |(\lambda - \lambda_{n_k})(x_{n_k})| \\ &= |\lambda_{n_k}(x_{n_k})| \geq \|\lambda_{n_k}\|/2 \end{aligned}$$

which implies $\|\lambda_{n_k}\| \to 0$ as $k \to \infty$. Thus $\lambda = 0$ which is a contradiction. Therefore $\mathscr{D}$ is dense and X is separable. ∎

The example of ℓ_1 and ℓ_∞ shows that the converse of this theorem does not hold. Incidently, Theorem III.7 provides a proof that ℓ_1 is not the dual of ℓ_∞, since ℓ_1 is separable and ℓ_∞ is not.

III.4 Operations on Banach spaces

We have already seen several ways in which new Banach spaces can arise from old ones. The successive duals of a Banach space are Banach spaces and the bounded operators from one Banach space to another form a Banach space. Also, any closed linear subspace of a Banach space is a Banach space. There are two other ways of constructing new Banach spaces which we will need: direct sums and quotient spaces.

Let A be an index set (not necessarily countable), and suppose that for each $\alpha \in A$, X_α is a Banach space. Let

$$X = \{\{x_\alpha\}_{\alpha \in A} \mid x_\alpha \in X_\alpha, \ \sum_{\alpha \in A} \|x_\alpha\|_{X_\alpha} < \infty\}$$

Then X with the norm

$$\|\{x_\alpha\}\| = \sum_{\alpha \in A} \|x_\alpha\|_{X_\alpha}$$

is a Banach space. It is called the **direct sum** of the spaces X_α and is often written $X = \bigoplus_{\alpha \in A} X_\alpha$. We remark that the Hilbert space direct sum and the Banach space direct sum are not necessarily the same. For example, if we take a countable number of copies of $\mathbb{C}$, the Banach space direct sum is ℓ_1, while the Hilbert space direct sum is ℓ_2. However, if one has a *finite* number of Hilbert spaces, their Hilbert space direct sum and their Banach space direct sum are isomorphic in the sense of Section III.1.

Let M be a closed linear subspace of a Banach space X. If X were a Hilbert space, we could write $X = M \oplus M^\perp$. The Banach space that we now define can sometimes take the place of $M^\perp$ in the Banach space case where there is no orthogonality. If x and y are elements of X, we will write $x \sim y$ if $x - y \in M$. The relation $\sim$ is an equivalence relation; we denote the set of equivalence classes by X/M. As usual we denote the equivalence class containing x by $[x]$. We define addition and scalar multiplication of equivalence classes by

$$\alpha[x] + \beta[y] = [\alpha x + \beta y]$$

which makes sense since the equivalence class on the right only depends on the equivalence classes from which x and y are chosen, not on the elements themselves. With these operations X/M, becomes a complex vector space (the class M is the zero element). Now define

$$\|[x]\|_1 = \inf_{m \in M} \|x - m\|_X$$

It is not hard to show that $\|\cdot\|_1$ is a norm on X/M. $\|[x]\| = 0$ implies $[x] = 0$ because M is closed. We will show that X/M with this norm is complete by using Theorem III.3. Let $\{[x_n]\}_{n=1}^{\infty}$, be an absolutely summable sequence in X/M. That is,

$$\sum_{n=1}^{\infty} \inf_{m \in M} \|x_n - m\| < \infty$$

For each n, choose $m_n \in M$ so that

$$\|x_n - m_n\| \leq 2 \inf_{m \in M} \|x_n - m\|$$

Then $\{x_n - m_n\}$ is absolutely summable in X. Since X is complete, $\{x_n - m_n\}$ is summable. Let

$$y = \lim_{N \to \infty} \sum_{n=1}^{N} (x_n - m_n)$$

Then

$$\left\| \sum_{n=1}^{N} [x_n] - [y] \right\|_1 \leq \left\| \sum_{n=1}^{N} x_n - y - \sum_{n=1}^{N} m_n \right\| \to 0 \quad \text{as } N \to \infty$$

This proves that $\{[x_n]\}$ is summable. Using Theorem III.3 again we conclude that X/M is complete. X/M is called the **quotient space** of X by M. The reader should work out the easy details of the following example.

Example Let $X = C[0, 1]$ and let $M = \{f \mid f(0) = 0\}$. Then $X/M = \mathbb{C}$.

III.5 The Baire category theorem and its consequences

Many questions in Banach space theory involve proving that sets have nonempty interiors. For example:

Proposition Let X and Y be normed linear spaces. Then a linear map $T: X \to Y$ is bounded if and only if

$$T^{-1}[\{y \mid \|y\|_Y \leq 1\}]$$

has a nonempty interior.

Proof Suppose that T is given and the set in question contains the ball

$$\{x \mid \|x - x_0\|_X < \varepsilon\}$$

Then $\|x\| < \varepsilon$ implies

$$\|Tx\| \leq \|T(x + x_0)\| + \|Tx_0\| \leq 1 + \|T(x_0)\|$$

since $x + x_0$ is in the ball of radius ε about x_0. Thus for all $x \in X$,

$$\|Tx\| \leq \varepsilon^{-1}(\|Tx_0\| + 1)\|x\|$$

so T is bounded. The converse is easy. ∎

It is thus of great interest to know when sets must have nonempty interiors. There is an extraordinary theorem about complete metric spaces. Before stating it, we make the following definition.

Definition A set S in a metric space M is called **nowhere dense** if $\bar{S}$ has an empty interior.

Theorem III.8 (Baire category theorem) A complete metric space is never the union of a countable number of nowhere dense sets.

Proof The idea of the proof is simple. Suppose that M is the complete metric space and $M = \bigcup_{n=1}^{\infty} A_n$ with each A_n nowhere dense. We will construct a Cauchy sequence $\{x_m\}$ which stays away from each A_n so that its limit point x (which is in M by completeness) is in no A_n, thereby contradicting the statement $M = \bigcup_{n=1}^{\infty} A_n$.

Since A_1 is nowhere dense, we can find $x_1 \notin \bar{A}_1$. Pick an open ball B_1 about x_1 so that $B_1 \cap A_1 = \varnothing$ and so that the radius of B_1 is smaller than one. Since A_2 is nowhere dense, we can find $x_2 \in B_1 \backslash \bar{A}_2$. Let B_2 be an open ball about x_2 so that $\bar{B}_2 \subset B_1$, $B_2 \cap A_2 = \varnothing$, and with radius smaller than $\frac{1}{2}$. Proceeding inductively, we pick $x_n \in B_{n-1} \backslash \bar{A}_n$ and choose an open ball B_n about x_n satisfying $\bar{B}_n \subset B_{n-1}$, $B_n \cap A_n = \varnothing$, and having a radius smaller than 2^{1-n}. Now $\{x_n\}_{n=1}^{\infty}$ is a Cauchy sequence since $n, m \geq N$ implies that x_n, $x_m \in B_N$ so

$$\rho(x_n, x_m) \leq 2^{1-N} + 2^{1-N} = 2^{2-N} \to 0$$

as $N \to \infty$. Let $x = \lim_{n\to\infty} x_n$. Since $x_n \in B_N$ for $n \geq N$, we have

$$x \in \bar{B}_N \subset B_{N-1}$$

Thus $x \notin A_{N-1}$ for any N which contradicts $M = \bigcup_{n=1}^{\infty} A_n$. ∎

The Baire category theorem tells us that if $M = \bigcup_{n=1}^{\infty} A_n$, then some of the sets $\bar{A}_n$ must have nonempty interior. In practice, one rarely uses the Baire category theorem directly but rather one of the following consequences. The first is known as the Banach–Steinhaus theorem or the principle of uniform boundedness.

Theorem III.9 (principle of uniform boundedness) Let X be a Banach space. Let $\mathscr{F}$ be a family of bounded linear transformations from X to some normed linear space Y. Suppose that for each $x \in X$, $\{\|Tx\|_Y \mid T \in \mathscr{F}\}$ is bounded. Then $\{\|T\| \mid T \in \mathscr{F}\}$ is bounded.

Proof Let $B_n = \{x \mid \|Tx\| \leq n \text{ for all } T \in \mathscr{F}\}$. By the hypothesis each x is in some B_n, that is, $X = \bigcup_{n=1}^{\infty} B_n$. Moreover each B_n is closed (since each T is continuous). By the Baire category theorem, some B_n has a nonempty interior. By mimicking the argument in the proposition at the beginning of this section, we conclude that the $\|T\|$'s are uniformly bounded. ∎

As a typical application of this theorem we have (see also Problem 13):

Corollary Let X and Y be Banach spaces and let $B(\cdot, \cdot)$ be a separately continuous bilinear mapping from $X \times Y$ to $\mathbb{C}$, that is, for each fixed x, $B(x, \cdot)$ is a bounded linear transformation, and for each fixed y, $B(\cdot, y)$ is a bounded linear transformation. Then $B(\cdot, \cdot)$ is jointly continuous, that is, if $x_n \to 0$ and $y_n \to 0$ then $B(x_n, y_n) \to 0$.

Proof Let $T_n(y) = B(x_n, y)$. Since $B(x_n, \cdot)$ is continuous, each T_n is bounded. Since $x_n \to 0$ and $B(\cdot, y)$ is bounded, $\{\|T_n(y)\|\}$ is bounded for each fixed y. Therefore, there exists C so that

$$\|T_n(y)\| \leq C\|y\|$$

for all n. Thus

$$\|B(x_n, y_n)\| = \|T_n(y_n)\| \leq C\|y_n\| \to 0$$

as $n \to \infty$. ∎

We remark that even on $\mathbb{R}^2$, for nonlinear functions separate continuity does not imply joint continuity. The standard example is

$$f(x, y) = \frac{xy}{x^2 + y^2} \qquad \text{if} \quad \langle x, y \rangle \neq \langle 0, 0 \rangle$$

$$f(0, 0) = 0$$

The second application of the Baire category theorem is to the following series of results.

Theorem III.10 (open mapping theorem) Let $T: X \to Y$ be a bounded linear transformation of one Banach space *onto* another Banach space Y. Then if M is an open set in X, $T[M]$ is open in Y.

Proof We make a series of remarks which will simplify the proof. We need only show that, for every neighborhood N of x, $T[N]$ is a neighborhood of $T(x)$. Since $T[x + N] = T(x) + T[N]$ we need only show this for $x = 0$. Since neighborhoods contain balls it is sufficient to show that $T[B_r^X] \supset B_{r'}^Y$ for some r' where

$$B_r^X = \{x \in X \mid \|x\| < r\}$$

However, since $T[B_r^X] = rT[B_1^X]$, we need only show that $T[B_r^X]$ is a neighborhood of zero for some r. Finally, by the "translation argument" of the proposition, it is sufficient to show that $T[B_r^X]$ has a nonempty interior for some r.

Since T is onto,

$$Y = \bigcup_{n=1}^{\infty} T[B_n]$$

so some $\overline{T(B_n)}$ has a nonempty interior. Now the hard work begins, since we want $T(B_n)$ to have a nonempty interior. By scaling and translating we can suppose that B_ε is contained in $\overline{T[B_1]}$; we will show that $\overline{T[B_1]} \subset T[B_2]$ which will complete the proof.

Let $y \in \overline{T[B_1]}$. Pick $x_1 \in B_1$ so $y - Tx_1 \in B_{\varepsilon/2} \subset \overline{T[B_{1/2}]}$. Now pick $x_2 \in B_{1/2}$ so that

$$y - Tx_1 - Tx_2 \in B_{\varepsilon/4}$$

By induction, we choose $x_n \in B_{2^{1-n}}$ so that

$$y - \sum_{j=1}^{n} Tx_j \in B_{\varepsilon 2^{1-n}}$$

Then $x = \sum_{i=1}^{\infty} x_i$ exists and is in B_2 and

$$y = \sum_{j=1}^{\infty} Tx_i = Tx$$

Thus $y \in T[B_2]$. ∎

Theorem III.11 (inverse mapping theorem) A continuous bijection of one Banach space onto another has a continuous inverse.

Proof T is open so T^{-1} is continuous. ∎

For an application of this result see Problem 19.

Definition Let T be a mapping of a normed linear space X into a normed linear space Y. The **graph** of T, denoted by $\Gamma(T)$, is defined as

$$\Gamma(T) = \{\langle x, y\rangle \mid \langle x, y\rangle \in X \times Y, \quad y = Tx\}$$

Theorem III.12 (closed graph theorem) Let X and Y be Banach spaces and T a linear map of X into Y. Then T is bounded if and only if the graph of T is closed.

Proof Suppose that $\Gamma(T)$ is closed. Then, since T is linear, $\Gamma(T)$ is a subspace of the Banach space $X \oplus Y$. By assumption $\Gamma(T)$ is closed and thus is a Banach space in the norm

$$\|\langle x, Tx\rangle\| = \|x\| + \|Tx\|$$

Consider the continuous maps Π_1, Π_2,

$$\Pi_1 : \langle x, Tx\rangle \to x, \qquad \Pi_2 : \langle x, Tx\rangle \to Tx$$

Π_1 is a bijection so by the inverse mapping theorem Π_1^{-1} is continuous. But $T = \Pi_2 \circ \Pi_1^{-1}$, so T is continuous. The converse is trivial. ∎

To avoid future confusion, we emphasize that the T in this theorem is implicitly assumed to be defined on all of X. We will later deal with transformations defined on *algebraic* subspaces of X (not all of X) with closed graphs which are not continuous. To appreciate what the closed graph theorem really does, consider the three statements:

(a) x_n converges to some element x.
(b) Tx_n converges to some element y.
(c) $Tx = y$.

In metric spaces, one sometimes says something is "true almost everywhere" if it is true on a residual; thereby, first category sets play the role of "sets of measure zero". There are some amusing results on this notion of a.e. in G. Choquet's book, *Lectures in Analysis*, Vol. I, pp. 120–126, Benjamin, New York, 1969. Warning: There exist sets $X \subset [0, 1]$ which are first category with measure 1! Thus the two notions of a.e., Lebesgue and Baire, are quite different.

Other topological spaces besides complete metric spaces have the property that residuals are dense; such spaces are called Baire spaces. For example, every locally compact space is Baire. For additional discussion, see Choquet's book, pp. 105–120.

PROBLEMS

†*1.* Prove that $L^\infty(\mathbb{R})$ is a Banach space.

†*2.* (a) Prove that ℓ_p and c_0 are separable but ℓ_∞ is not.
(b) Prove that $s \subset \ell_p$ for all p.

†*3.* Prove that a normed linear space is complete if and only if every absolutely summable sequence is summable. (Hint for the "if" part: To show that a Cauchy sequence converges it is only necessary to show that a subsequence converges.)

**4.* Prove that all norms on $\mathbb{R}^n$ are equivalent. (Hint: Use the fact that the unit sphere is compact in the Euclidean topology.)

†*5.* Prove that $C_\infty(\mathbb{R})$ is the completion of $\kappa(\mathbb{R})$.

6. Prove that if $\{\lambda_k\}_{k=1}^\infty \in \ell_1$ then the linear functional on c_0 given by

$$\Lambda(\{a_k\}_{k=1}^\infty) = \sum \lambda_k a_k$$

has norm $\sum_{k=1}^\infty |\lambda_k|$.

7. Prove that $\ell_\infty = \ell_1^*$ but that $\ell_\infty^* \neq \ell_1$ by using the Hahn–Banach theorem.

8. (a) Prove that there is a nonzero bounded linear functional on $L^\infty(\mathbb{R})$ which vanishes on $C(\mathbb{R})$.
(b) Prove that there is a bounded linear functional λ on $L^\infty(\mathbb{R})$ such that $\lambda(f) = f(0)$ for each $f \in C(\mathbb{R})$.

9. Suppose that $\mathscr{H}$ is a Hilbert space and that λ is a bounded linear functional on $\mathscr{M}$, a not necessarily closed subspace. Describe the continuous extensions of λ.

†*10.* Prove the third corollary to the Hahn–Banach theorem.

11. Prove that there is a linear functional λ on $\ell_\infty(\mathbb{R})$ so that

$$\underline{\lim}_{n\to\infty} a_n \leq \lambda(\{a_n\}_{n=1}^\infty) \leq \overline{\lim}_{n\to\infty} a_n$$

$\ell_\infty(\mathbb{R}) = \{a \mid a \in \ell_\infty, \quad a_n \in \mathbb{R} \quad \text{for all } n\}$.

†*12.* Prove the statement in the example at the end of Section 4.

13. Use the uniform boundedness principle to provide an alternative proof of the Hellinger–Toeplitz theorem.

**14.* Let X be a Banach space. Give an example of an everywhere-defined but discontinuous linear functional λ. Show directly that λ is not closed.

15. Let $\mathscr{H}$ be a separable Hilbert space with an orthonormal basis $\{x_n\}_{n=1}^{\infty}$. Let $\{y_n\}$ be a sequence of elements of $\mathscr{H}$ and prove that the following two statements are equivalent.

(a) $(x, y_n) \underset{n\to\infty}{\to} 0$, $\forall x \in \mathscr{H}$.

(b) $(x_m, y_n) \underset{n\to\infty}{\to} 0$, for each $m = 1, 2, \ldots$, and $\{\|y_n\|\}_{n=1}^{\infty}$ is bounded.

16. A subset S of a Banach space is called **weakly bounded** if and only if for all $\lambda \in X^*$, $\sup_{x\in S} |\lambda(x)| < \infty$. S is called **strongly bounded** if and only if $\sup_{x\in S} \|x\| < \infty$. Prove that a set is strongly bounded if and only if it is weakly bounded (see Section V.7).

17. Prove that a separately continuous multilinear functional on a Banach space is jointly continuous.

18. Extend the Hellinger–Toeplitz theorem to include pairs of operators A, B satisfying: $(Ax, y) = (x, By)$.

19. Let X be a Banach space in either of the norms $\|\cdot\|_1$ or $\|\cdot\|_2$. Suppose that $\|\cdot\|_1 \leq C\|\cdot\|_2$ for some C. Prove that there is a D with $\|\cdot\|_2 \leq D\|\cdot\|_1$.

20. Why doesn't a one-point space violate the Baire theorem?

**21.* Prove that any countable intersection of dense open sets in a complete metric space is dense.

22. (a) Prove that a Banach space X is reflexive if and only if X^* is reflexive. (Hint: If $X \neq X^{**}$ find a bounded linear functional on X^{**} which vanishes on X).
(b) Prove that whenever X is a nonreflexive Banach space, $(\cdots(X^*)^*\cdots)^*$ is not reflexive.

23. Let X be a Hilbert space and let $\mathscr{M}$ be a closed subspace. Show that the restriction of the natural map $\pi : X \to X/\mathscr{M}$ is an isomorphism of $\mathscr{M}^{\perp}$ and $X/\mathscr{M}$.

24. Let ℓ be a linear functional on a real Banach space X. Prove that $X/\ker \ell$ is isomorphic to $\mathbb{R}$ with the usual norm and that the natural projection $\pi : X \to X/\ker \ell = \mathbb{R}$ is related to ℓ by $\ell = \pm \|\ell\|\pi$.

25. A Banach space is called **uniformly convex** if for each $\varepsilon > 0$, there is a $\delta > 0$, so that $\|x\| = \|y\| = 1$ and $\|\frac{1}{2}(x + y)\| > 1 - \delta$ imply $\|x - y\| < \varepsilon$; thus the unit ball is uniformly round. We will see in Problem 15 of Chapter V, that every uniformly convex space is reflexive.

A priori, to prove that T is continuous one must show that (a) implies (b) and (c). What the closed graph theorem says is that it is sufficient to prove that (a) and (b) imply (c).

The following corollary of the closed graph theorem has important consequences in mathematical physics.

Corollary (the Hellinger–Toeplitz theorem) Let A be an everywhere-defined linear operator on a Hilbert space $\mathscr{H}$ with $(x, Ay) = (Ax, y)$ for all x and y in $\mathscr{H}$. Then A is bounded.

Proof We will prove that $\Gamma(A)$ is closed. Suppose that $\langle x_n, Ax_n\rangle \to \langle x, y\rangle$. We need only prove that $\langle x, y\rangle \in \Gamma(A)$, that is, that $y = Ax$. But, for any $z \in \mathscr{H}$,

$$(z, y) = \lim_{n\to\infty} (z, Ax_n) = \lim_{n\to\infty} (Az, x_n)$$
$$= (Az, x) = (z, Ax)$$

Thus $y = Ax$ and $\Gamma(A)$ is closed. ∎

As we shall see, this theorem is the cause of much technical pain because in quantum mechanics there are operators (like the energy) which are unbounded but which we want to obey

$$(x, Ay) = (Ax, y)$$

in some sense. The Hellinger–Toeplitz theorem tells us that such operators cannot be everywhere defined. Thus such operators are defined on subspaces $D(A)$ of $\mathscr{H}$ and defining what one means by $A + B$ or AB may be difficult. For example, $A + B$ is a priori only defined on $D(A) \cap D(B)$ which may equal $\{0\}$ even in the case where both $D(A)$ and $D(B)$ are dense. We return to these questions in Chapters VIII and X.

NOTES

Section III.1 The name Banach space honors the important work of S. Banach on normed linear spaces during the 1920's culminating in his book, *Théorie des Opérations Linéaires*, Monografie Math., I, Warsaw, 1932. A good elementary reference for the material in this chapter is the book *Foundations of Modern Analysis* by A. Friedman, Holt, New York, 1970. In the second supplement we prove Hölder's inequality only in the case $r = 1$. To prove the general case where $p^{-1} + q^{-1} = r^{-1}$ observe that

$$|fg|^r = |f|^r |g|^r$$

and use the Hölder inequality for the special case where

$$\frac{1}{(p/r)} + \frac{1}{(q/r)} = 1$$

obtaining

$$\int |fg|^r \leq \left(\int |f|^{rp/r}\right)^{r/p} \left(\int |g|^{rq/r}\right)^{r/q}$$

or

$$\left(\int |fg|^r\right)^{1/r} \leq \left(\int |f|^p\right)^{1/p} \left(\int |g|^q\right)^{1/q}$$

Suppose X is a Banach space. One of the ways of studying the Banach space of operators from X to itself, $\mathscr{L}(X, X)$, is to use the fact that it is also an algebra. Thus, one can use algebraic notions like ideals and commutators to investigate the structure of $\mathscr{L}(X, X)$. In Section VI.6 certain important ideals of $\mathscr{L}(\mathscr{H}, \mathscr{H})$, where $\mathscr{H}$ is a separable Hilbert space, are studied. The general theory of operator algebras is studied in later volumes.

Section III.2 The proof that $(L^p)^* = L^q$ may be found in Royden's book (see the Notes for Chapter I) or may be proven using the notion of uniformly convex space (see Problems 25 and 26 of Chapter III and Problem 15 of Chapter V). In Section VI.6 we discuss the duals of several subalgebras of $\mathscr{L}(\mathscr{H}, \mathscr{H})$.

Section III.3 The Hahn–Banach theorem dates back to the work of Helly in "Über Lineare Funktional Operationen," *Sitzgsber, Akad. Wiss. Wien Math-Nat. Kl.* **121 IIa**, (1912), 265–297, and "Über Systeme linearer Gleichungen mit Unendlich Vielen Unbekannten," *Monatsh. Math. Phys.* 31, (1921), 60–91. The modern version is due to H. Hahn, "Über lineare Gleichungssystem in linearen Räumen," *J. Reine Angew. Math.* **157**, (1926), 214–229, and S. Banach, "Sur les fonctionelles linéaires, I, II," *Studia Math.* **1** (1929), 211–216, 223–239. A nice example of the concrete applications of the Hahn–Banach theorem may be found in the book by Friedman mentioned above. There it is shown how to use the Hahn–Banach theorem to prove the existence of a Green's function for the Dirichlet problem in two dimensions.

Section III.5 The Baire theorem was proven in R. Baire, "Sur les fonctions de variables réelles," *Annali di Mat. Ser. 3* **3** (1899), 1–123. The general case is in C. Kuratowski, "La propriété de Baire dans les espaces métriques," *Fund. Math.* **16** (1930), 390–394, and S. Banach, "Théorèmes sur les ensembles de premières catégorie," *Fund. Math.* **16**, (1930), 395–398. The Banach–Steinhaus theorem was proven by S. Banach and H. Steinhaus in "Sur le principe de la condensation de singularités." *Fund. Math.* **9**, (1927), 50–61. There is a discussion of the Baire theorem and its consequences in Lorch's book (see the Notes for Section II.5). The term category comes from the following: A countable union of nowhere dense sets is called a **first category** set. All other sets are called **second category**. The Baire theorem says that any complete metric space is second category.

Complements of first category sets are often called residuals. A residual set is thus a set containing a countable intersection of dense open sets. The Baire theorem implies that any residual in a complete metric space is dense (Problem 21).

(a) Prove directly that $L^1(\mathbb{R})$ and $L^\infty(\mathbb{R})$ are not uniformly convex.
(b) Prove that any Hilbert space is uniformly convex.
*(c) Prove that $L^p(X, d\mu)$ is uniformly convex for $p \geq 2$. Hint: Prove that for $\alpha, \beta \in \mathbb{C}$, one has $|\alpha+\beta|^p + |\alpha-\beta|^p \leq 2^{p-1}(|\alpha|^p + |\beta|^p)$ by first proving

$$(|\alpha+\beta|^p + |\alpha-\beta|^p)^{1/p} \leq \sqrt{2}(|\alpha|^2 + |\beta|^2)^{1/2}$$

Notes: 1. L^p is actually uniformly convex for all $1 < p < \infty$, but the proof for $1 < p < 2$ is harder; c.f. G. Köthe: *Topological Vector Spaces, I*, Springer (1969), 358–359.
2. Uniformly convex spaces were introduced by J. Clarkson, "Uniformly convex spaces," *Trans. A.M.S.* **40** (1936), 396–414.
3. M. Day has given examples of reflexive Banach spaces which are not uniformly convex in "Reflexive Banach spaces not isomorphic to uniformly convex spaces," *Bull. A.M.S.* **47** (1941), 313–317; see also Köthe, pp. 360–363.

26. (a) A pair of Banach spaces, X and Y, are said to be in **strict duality** if there is a map $f: X \to Y^*$ which is isometric, so that the induced map $f^*: Y \to X^*$ is also isometric. Prove that if X and Y are in strict duality and X is reflexive, then $Y = X^*$ and $X = Y^*$. (Hint: Use the Hahn–Banach theorem.)
(b) Prove that $L^p(X, d\mu)$ and $L^q(X, d\mu)$ are in strict duality if $p^{-1} + q^{-1} = 1$.
(c) Prove that $L^p(X, d\mu)^* = L^q(X, d\mu)$ if $1 < p < \infty$ and $p^{-1} + q^{-1} = 1$. (Hint: Use Problem 25 and Problem 15 of Chapter V).

*27. Prove the Banach–Schauder theorem: Let T be a continuous linear map, $T: E \to F$, where E and F are Banach spaces. Then either $T[A]$ is open in $T[E]$ for each open $A \subset E$, or $T[E]$ is of first category in $\overline{T[E]}$ (see the notes to Section 5 for the definition of first category).

28. (a) Prove that every quotient of ℓ_2 by a closed subspace is isometrically isomorphic to either ℓ_2 or $\mathbb{C}^N$ for some N.
(b) Prove that ℓ_1 is not topologically isomorphic to any quotient space of ℓ_2.

29. Let X be a separable Banach space. Let $\{x_1, \ldots, x_n, \ldots\}$ be a dense subset of the unit ball in X. Map $\ell_1 \to X$ by

$$A: \langle \alpha_1, \ldots, \alpha_n, \ldots \rangle \to \sum_{n=1}^{\infty} \alpha_n x_n$$

(a) Prove that A is well defined and continuous.
(b) Prove that Ker A is closed and that A "lifts" to a continuous map $\hat{A}: \ell_1/\text{Ker } A \to X$.
(c) Prove Ran $\hat{A}$ = Ran A is all of X. Hint: Given x with $\|x\| = 1$, choose $x_{n(i)}$ recursively by requiring

$$\left\| x - \sum_{i=1}^{k} 2^{-i+1} x_{n(i)} \right\| \leq 2^{-k}$$

(d) Conclude that any separable Banach space is topologically isomorphic to some quotient space of ℓ_1.
(e) By using (c) with 2 replaced by $3, 4, \ldots$, show that $\hat{A}$ is actually an isometry.

30. Let X be a Banach space and let Y be a closed subspace of X. Let Y° in X^* be defined by

$$Y^\circ = \{\ell \in X^* | \ell \restriction Y = 0\}$$

Given a bounded linear functional f on X/Y, define $\pi^*(f) \in X^*$ by $[\pi^*(f)](x) = f([x])$. Prove that π^* is an isometric isomorphism of $(X/Y)^*$ onto Y°.

31. (a) Let E be a Banach space with separable dual and $\langle M, \mu\rangle$ a measure space with $L^p(M, d\mu)$ separable for all $1 < p < \infty$. Develop the theory of $L^p(M, d\mu; E)$ analogous to the theory of $L^2(M, d\mu; \mathscr{H})$ discussed in Sections II.1 and II.4.

(b) Prove $L^p(M \times N, d\mu \otimes d\nu)$ and $L^p(M, d\mu; L^p(N, d\nu))$ are naturally isomorphic.

*(c) Let E^{**} be a separable Banach space and let $1 \leq p < \infty$. Prove that $L^p(M, d\mu, E)^*$ is naturally isometrically isomorphic to $L^q(M, d\mu, E^*)$ (Hint: First show that it is enough to prove that every bounded linear transformation T of E into $L^q(M, d\mu)$ is of the form $[T(x)](m) = [f(m)](x)$ for some $f \in L^q(M, d\mu; E^*)$. Prove this in the special case where $E = \ell_1$. Finally use Problems 29 and 30 to treat the general separable Banach space, E.)

**32.* Let S be a closed linear subspace of $L^1[0, 1]$. Suppose that $f \in S$ implies that $f \in L^p[0, 1]$ for some $p > 1$. Prove that $S \subset L^p[0, 1]$ for some $p > 1$.

IV: Topological Spaces

Everyone knows what a curve is, until he has studied enough mathematics to become confused through the countless number of possible exceptions. *F. Klein*

IV.1 General notions

The abstract notions of limit and convergence are the bread and butter of functional analysis. The purely metric space formulations that we have used thus far are sadly lacking in some cases, so it is necessary to introduce more general concepts. It is possible to describe what is known as a topological space purely in terms of convergence, but it is very awkward. Instead, one usually defines a topological space by abstracting the notion of open sets in metric spaces. Convergence then becomes a derived concept. We discuss convergence in Section IV.2.

This section consists primarily of definitions as we introduce an extensive language needed to describe topological notions. We urge the reader to learn the language by returning to this section when necessary rather than by brute memorization.

Definition A **topological space** is a set S with a distinguished family of subsets $\mathscr{T}$ called **open sets** with the properties:

(i) $\mathscr{T}$ is closed under finite intersections, that is, if $A, B \in \mathscr{T}$, then $A \cap B \in \mathscr{T}$.

(ii) $\mathscr{T}$ is closed under *arbitrary* unions, that is, if $A_\alpha \in \mathscr{T}$ for all α in some index set I, then $\bigcup_{\alpha \in I} A_\alpha \in \mathscr{T}$.
(iii) $\varnothing \in \mathscr{T}$ and $S \in \mathscr{T}$.

$\mathscr{T}$ is called a **topology** for S. We will occasionally write $\langle S, \mathscr{T} \rangle$ for a topological space.

In contradistinction to Borel structure, topological structures are *not* symmetric between intersection and union and involve not merely countable operations but arbitrary operations.

The prime example of a topological space is a metric space. The open sets, $\mathscr{T}$, are those sets, $M \subset S$, with the property $(\forall x \in M)(\exists r > 0)$ $\{y | \rho(x, y) < r\} \subset M$. After discussing continuous functions, we will describe another family of examples. We first mention, however, two trivial examples: Given a set S, the family of all subsets of S is a topology; it is called the discrete topology. $\mathscr{T} = \{\varnothing, S\}$ is also a topology; it is called the indiscrete topology.

The family of all topologies on a set S is ordered in a natural way $\mathscr{T}_1 \prec \mathscr{T}_2$ if $\mathscr{T}_1 \subset \mathscr{T}_2$ in the sense of set-theoretic inclusion. If $\mathscr{T}_1 \prec \mathscr{T}_2$, we say $\mathscr{T}_1$ is a **weaker** topology than $\mathscr{T}_2$. (The term weaker comes from the fact that more sequences converge in $\mathscr{T}_1$ than in $\mathscr{T}_2$; so $\mathscr{T}_1$ convergence is a weaker notion than $\mathscr{T}_2$ convergence.)

Definition A family $\mathscr{B} \subset \mathscr{T}$ is called a **base** if and only if any $T \in \mathscr{T}$ is of the form $T = \bigcup_\alpha B_\alpha$ for some family $\{B_\alpha\} \subset \mathscr{B}$.

For example, the balls in a metric space are always a base. We now take a whole family of definitions directly from metric spaces:

Definition A set N is called a **neighborhood** of a point $x \in S$, a topological space, if there exists an open set U with $x \in U \subset N$.

A family $\mathscr{N}$ of subsets of S, a topological space, is called a **neighborhood base at** x if each $N \in \mathscr{N}$ is a neighborhood of x and if given any neighborhood M of x, there is an $N \in \mathscr{N}$ with $N \subset M$. Equivalently, $\mathscr{N}$ is a neighborhood base at x if and only if $\{M | N \subset M$ for some $N \in \mathscr{N}\}$ is the family of all neighborhoods of x. For example, if $\mathscr{B}$ is a base for $\mathscr{T}$, $\{N \in \mathscr{B} | x \in N\}$ is a neighborhood base at x. We emphasize that neighborhoods need not be open. In a metric space, the *closed* balls of radius greater than zero are a neighborhood base.

Definition A set $C \subset S$, a topological space, is called **closed** if and only if it is the complement of an open set.

The properties of the family of all closed sets can be read off from the properties of $\mathcal{T}$.

Definition Let $A \subset S$, a topological space. The **closure of** A, $\bar{A}$, is the smallest closed set containing A. The **interior of** A, A°, is the largest open set contained in A. The **boundary** of A is the set $\bar{A} \backslash A^\circ \equiv \bar{A} \cap \overline{[S \backslash A]}$.

That a smallest closed set containing A exists follows from the fact that $\mathcal{T}$ is closed under arbitrary unions.

As examples, we consider several topologies on $\mathbb{R}^2$:

Example 1 The ordinary metric topology.

Example 2 Consider the family of sets of the form $\{\langle x, y\rangle \mid x \in O\}$ where y is *fixed* and O is an open set of $\mathbb{R}$ in the usual topology. This family of sets is the base for a topology whose open sets are the sets C such that for each $y \in \mathbb{R}$, $\{x \mid \langle x, y\rangle \in C\}$ is open in $\mathbb{R}$ in the usual topology. In an intuitive sense, which we shall shortly make precise, this topology is the "product" of the usual topology in one factor and the discrete topology in the other factor.

Example 3 Let $\mathcal{T}$ consist of the empty set and all sets containing $\langle 0, 0\rangle$. A neighborhood base for $\langle x, y\rangle$ in this topology is the single (!) set $\{\langle 0, 0\rangle, \langle x, y\rangle\}$.

Our experience with metric spaces suggests that continuous functions will play a major role.

Definition Let $\langle S, \mathcal{T}\rangle$ and $\langle T, \mathcal{U}\rangle$ be two topological spaces. A function $f: S \to T$ is called **continuous** if $f^{-1}[A] \in \mathcal{T}$ for every $A \in \mathcal{U}$; that is, if the inverse image of any open set is open. f is called **open** if $f[B]$ is open for each $B \in \mathcal{T}$. If f is open and continuous, it is called **bicontinuous**. A bicontinuous bijection is called a **homeomorphism**.

Homeomorphisms are the "isomorphisms" of topological spaces. A topological notion is some notion (or object) invariant under homeomor-

phism. As an example, the intervals $(-\infty, \infty)$ and $(-1, 1)$ are homeomorphic under the homeomorphism $x \mapsto x/(1 + x^2)$. They are not isometric in the usual metric; in fact, only one of them is complete. This demonstrates that completeness is not a topological notion. However, most metric space notions that are useful in analysis are topological notions.

Continuity is often used to define topologies:

Definition Let $\mathscr{K}$ be a family of functions from a set S to a topological space $\langle T, \mathscr{U} \rangle$. The **$\mathscr{K}$-weak** (or simply **weak**) topology on S is the weakest topology for which all the functions $f \in \mathscr{K}$ are continuous.

To construct the $\mathscr{K}$-weak topology, take the family of all finite intersections of sets of the form $f^{-1}[U]$ where $f \in \mathscr{K}$ and $U \in \mathscr{U}$. These sets form a base for the $\mathscr{K}$-weak topology. If $\mathscr{K}$ is a family of functions on a set S but with values in different topological spaces, we define the $\mathscr{K}$-weak topology in the obvious way.

Example 4 Consider $C[a, b]$, the continuous functions on $[a, b]$. The **topology of pointwise convergence** on $C[a, b]$ is the weak topology given by the family of functions $f \mapsto f(x)$. That is, for each $x \in [a, b]$, let $E_x(f) = f(x)$ so the $E_x(\cdot)$ are maps of $C[a, b]$ to $\mathbb{R}$. As we will see, the topology of pointwise convergence is the topology on $C[a, b]$ for which $f_n \to f$ if and only if $f_n(x) \to f(x)$ for each x.

Example 5 Let $\mathscr{H}$ be a Hilbert space. The "weak topology" is the weakest topology making $\varphi \mapsto (\psi, \varphi)_{\mathscr{H}}$ continuous for each ψ in $\mathscr{H}$. A neighborhood base for 0 is given explicitly by the sets

$$N(\psi_1, \ldots, \psi_n; \varepsilon_1, \ldots, \varepsilon_n) = \{\varphi \mid |(\psi_i, \varphi)| < \varepsilon_i, \quad i = 1, \ldots, n\}$$

where $\varepsilon_i > 0$, $\psi_1, \ldots, \psi_n$ are arbitrary, and $n = 1, 2, \ldots$. Thus, the neighborhoods in the weak topology are cylinders in all but finitely many dimensions. That is, there is a subspace M (the orthogonal complement of $\psi_1, \ldots, \psi_n$) whose complement, $M^{\perp}$, is finite dimensional and so that $\varphi \in N, \eta \in M$ implies $\varphi + \eta \in N$.

Example 6 On $\mathbb{R}^2$ consider the maps π_1, π_2 given by $\pi_1(x, y) = x$; $\pi_2(x, y) = y$. The weak topology defined by π_1 and π_2 and the usual topology on $\mathbb{R}$ has rectangles $(a, b) \times (c, d)$ as a base for its open sets and thus the weak topology is the "usual" topology on $\mathbb{R}^2$.

Example 7 The weak topology can be used to topologize Cartesian products. Recall if $\{S_\alpha\}_{\alpha \in I}$ is a family of sets, $S = \prod_{\alpha \in I} S_\alpha$ is the family of all $\{x_\alpha\}_{\alpha \in I}$ with $x_\alpha \in S_\alpha$. For each α, we have a map $\pi_\alpha : S \to S_\alpha$ given by $\pi_\alpha(\{x_\beta\}_{\beta \in I}) = x_\alpha$. If each S_α has a topology $\mathcal{T}_\alpha$, we define the **product topology**, $\prod_{\alpha \in I} \mathcal{T}_\alpha$ as the weak topology generated by the projections π_α.

We now return to our listing of definitions by classifying spaces by how well open sets separate points and closed sets:

Definition

(a) A topological space is called a T_1 **space** if and only if for all x and y, $x \neq y$, there is an open set O with $y \in O$, $x \notin O$. Equivalently, a space is T_1 if and only if $\{x\}$ is closed for each x.

(b) A topological space is called **Hausdorff** (or T_2) if and only if for all x and y, $x \neq y$, there are open sets O_1, O_2 such that $x \in O_1$, $y \in O_2$, and $O_1 \cap O_2 = \varnothing$.

(c) A topological space is called **regular** (or T_3) if and only if it is T_1 and for all x and C, closed, with $x \notin C$, there are open sets O_1, O_2 such that $x_1 \in O_1$, $C \subset O_2$, and $O_1 \cap O_2 = \varnothing$. Equivalently, a space is T_3 if the closed neighborhoods of any point are a neighborhood base.

(d) A topological space is called **normal** (or T_4) if and only if it is T_1 and for all C_1, C_2, closed, with $C_1 \cap C_2 = \varnothing$, there are open sets O_1, O_2 with $C_1 \subset O_1$, $C_2 \subset O_2$, and $O_1 \cap O_2 = \varnothing$.

Obviously:

Proposition $T_4 \Rightarrow T_3 \Rightarrow T_2 \Rightarrow T_1$

We remark that the two most important notions are Hausdorff and normal. At this time, we avoid discussing another way of separating sets, namely with continuous functions. Urysohn's lemma (Theorem IV.7) deals with this question.

We next consider various countability criteria:

Definition

(i) A topological space S is called **separable** if and only if it has a countable dense set.

(ii) A topological space S is called **first countable** if and only if each point $x \in S$ has a countable neighborhood base.

(iii) A topological space S is called **second countable** if and only if S has a countable base.

The relation between these topological notions and metric spaces is set forward in the elementary:

Proposition (a) Every metric space is first countable.
(b) A metric space is second countable if and only if it is separable.
(c) Any second countable topological space is separable.

Warning There are separable spaces that are not second countable (see Problem 7). To add to the confusion, some authors use "separable" to mean second countable. *By separable we always mean that there exists a countable dense set.*

The geometric idea of being connected has a topological formulation:

Definition A topological space S is called **disconnected** if and only if it contains a nonempty proper subset, C, which is both open and closed; equivalently, S is disconnected if and only if it can be written as the union of two disjoint nonempty closed sets. If S is not disconnected, it is called **connected.**

We examine connectivity in Problems 3 and 6. As a final topological notion, we consider restricting topologies to subsets.

Definition Let $\langle S, \mathcal{T} \rangle$ be a topological space and let $A \subset S$. The **relative topology** on A is the family of sets $\mathcal{T}_A = \{O \cap A \mid O \in \mathcal{T}\}$. A subset $B \subset A$ is called **relatively open** if $B \in \mathcal{T}_A$ and **relatively closed** if $A \backslash B \in \mathcal{T}_A$.

IV.2 Nets and convergence

In this section we introduce new objects, called nets, in order to handle limit operations in general topological spaces. Although nets seem on first acquaintance to be bizarre, the propositions in this section show how natural they are.

Definition A **directed system** is an index set I together with an ordering $\prec$ which satisfies:

(i) If $\alpha, \beta \in I$, then there exists $\gamma \in I$ so that $\gamma \succ \alpha$ and $\gamma \succ \beta$.
(ii) $\prec$ is a partial ordering.

Definition A **net** in a topological space S is a mapping from a directed system I to S; we denote it by $\{x_\alpha\}_{\alpha \in I}$.

If we choose the positive integers with the usual order as a directed system, the nets on that directed system are just sequences in S, so nets are a generalization of the notion of sequence. If $P(\alpha)$ is a proposition depending on an index α in a directed set I we say $P(\alpha)$ is **eventually true** if there is a β in I with $P(\alpha)$ true if $\alpha \succ \beta$. We say $P(\alpha)$ is **frequently true** if it is not eventually false, that is, if for any β there is an $\alpha \succ \beta$ with $P(\alpha)$ true.

Definition A net $\{x_\alpha\}_{\alpha \in I}$ in a topological space S is said to **converge** to a point $x \in S$ (written $x_\alpha \to x$) if for any neighborhood N of x, there is a $\beta \in I$ so that $x_\alpha \in N$ if $\alpha \succ \beta$.

Thus $x_\alpha \to x$ if and only if x_α is eventually in any neighborhood of x. If x_α is frequently in any neighborhood of x, we say that x is a **cluster point** of $\{x_\alpha\}$. Notice that the notions of limit and cluster point generalize the same notions for sequences in a metric space.

Theorem IV.1 Let A be a set in a topological space S. Then, a point x is in the closure of A if and only if there is a net $\{x_\alpha\}_{\alpha \in I}$ with $x_\alpha \in A$, so that $x_\alpha \to x$.

Proof We first observe that $\bar{A}$ is just the set of points x such that any neighborhood of x contains a point of A. This set certainly contains A and its complement is the largest open set not containing any points of A. Now suppose $x_\alpha \to x$ where each $x_\alpha \in A$. Then any neighborhood of x contains some x_α and hence some points of A, that is, x is a limit point of A, so $x \in \bar{A}$.

Conversely, suppose $x \in \bar{A}$. Let I be the collection of neighborhoods of x with the ordering $N_1 \prec N_2$ if $N_2 \subset N_1$. For each $N \in I$, let x_N be a point in $A \cap N$. Then $\{x_N\}_{N \in I}$ is a net and $x_N \to x$. ∎

In spaces that are first countable, we can construct the closures of sets by using only sequences. Such is the case in metric spaces. The following example is a case where sequences are not enough:

Example Let $S = [0, 1]$; the nonempty open sets will be the subsets of $[0, 1]$ whose complements contain at most a countable infinity of points. Let $A = [0, 1)$. Then $\bar{A} = S$ since $\{1\}$ is not open. But, let $\{x_n\}_{n=1}^{\infty}$ be any sequence of points of $[0, 1)$. $\{x_n\}_{n=1}^{\infty}$ cannot converge to 1 since the complement of the points $\{x_n\}_{n=1}^{\infty}$ is an open set containing 1.

Although the above example seems artificial, spaces that are not first countable play a large role in functional analysis. Usually, they arise when dual spaces of Banach spaces are considered with topologies weaker than the norm topology (Section IV.5).

We state two facts about nets whose proofs are not difficult and are left as problems:

Theorem IV.2 (a) A function f from a topological space S to a topological space T is continuous if and only if for every convergent net $\{x_\alpha\}_{\alpha \in I}$ in S, with $x_\alpha \to x$, the net $\{f(x_\alpha)\}_{\alpha \in I}$ converges in T to $f(x)$.

(b) Let S be a Hausdorff space. Then a net $\{x_\alpha\}_{\alpha \in I}$ in S can have at most one limit; that is, if $x_\alpha \to x$ and $x_\alpha \to y$, then $x = y$.

Analogous to the concept of a subsequence we have the following definition:

Definition A net $\{x_\alpha\}_{\alpha \in I}$ is a **subnet** of a net $\{y_\beta\}_{\beta \in J}$ if and only if there is a function $F: I \to J$ such that

(i) $x_\alpha = y_{F(\alpha)}$ for each $\alpha \in I$.

(ii) For all $\beta' \in J$, there is an $\alpha' \in I$ such that $\alpha \succ \alpha'$ implies $F(\alpha) \succ \beta'$ (that is, $F(\alpha)$ is eventually larger than any fixed $\beta \in J$).

We then have the following proposition which shows that the above definition is the right one.

Proposition A point x in a topological space S is a cluster point of a net $\{x_\alpha\}$ if and only if some subnet of $\{x_\alpha\}$ converges to x.

Of course, subsequences are subnets of sequences. But it is also possible for a sequence in a topological space to have no convergent subsequences but to have convergent subnets (see Problem 12).

IV.3 Compactness †

The reader no doubt remembers the special role that closed bounded subsets of $\mathbb{R}^n$ played in elementary analysis. In this section we will study the topological abstraction of this concept:

† A supplement to this section begins on p. 351.

Definition We say a topological space $\langle S, \mathcal{T} \rangle$ is **compact** if any open cover of S has a finite subcover, that is, if for any family $\mathcal{U} \subset \mathcal{T}$ with $S = \bigcup_{U \in \mathcal{U}} U$, there is a finite subset $\{U_1, \ldots, U_n\} \subset \mathcal{U}$ with $S = \bigcup_{i=1}^n U_i$. A subset of a topological space is called a **compact set** if it is a compact space in the relative topology.

Henceforth in our discussion we will always suppose that all compact spaces are Hausdorff, although occasionally we will repeat this condition for emphasis.

Since we have a considerable amount of material to discuss, it is perhaps useful to describe briefly the contents of the next two sections. After studying some equivalent formulations of compactness and some elementary properties of compact spaces, we turn to some of the pillars of functional analysis. We first state and discuss Tychonoff's theorem. We then turn to the study of continuous functions on compact sets. After showing that a compact Hausdorff space X has lots of continuous functions (Urysohn's lemma), we discuss the Banach space $C(X)$ of continuous functions. We state the Stone–Weierstrass theorem but defer its instructive proof to an appendix. In the next section, we determine the dual of $C(X)$. Using the Riesz–Markov theorem, we will prove that $C(X)^*$ is identical with $\mathcal{M}(X)$, the family of signed measures on X.

We first reformulate the notion of compactness by taking complements of open sets:

Definition A topological space S is said to have the **finite intersection property** (f.i.p.) if and only if any family of closed sets $\mathcal{F}$ with $\bigcap_{i=1}^n F_i \neq \varnothing$ for any finite subfamily $\{F_i\}_{i=1}^n \subset \mathcal{F}$ satisfies $\bigcap_{F \in \mathcal{F}} F \neq \varnothing$.

Proposition (f.i.p. criterion) S is compact if and only if S has the f.i.p.

Proof Let $\mathcal{F}$ be given and let $\mathcal{U} = \{S \backslash F \mid F \in \mathcal{F}\}$. Then $\mathcal{F}$ has the property that $\bigcap_{i=1}^n F_i \neq \varnothing$ if and only if $\mathcal{U}$ has no finite subcover and the property that $\bigcap_{F \in \mathcal{F}} F \neq \varnothing$ if and only if $\mathcal{U}$ is not a cover. The reader is invited to wend his way through the double negatives to complete the proof. ∎

A somewhat deeper reformulation is:

Theorem IV.3 (The Bolzano–Weierstrass theorem) A space S is compact if and only if every net in S has a convergent subnet.

Proof Suppose that every net has a convergent subnet and let $\mathcal{U}$ be an open cover. Let us suppose that $\mathcal{U}$ has no finite subcover and derive a contradiction.

Order the finite subfamilies $\mathfrak{S}$ of $\mathscr{U}$ by inclusion; $\mathfrak{S}$ is thereby a directed set. For each $\mathscr{F} \equiv \{F_1, \ldots, F_m\} \in \mathfrak{S}$, pick $x_{\mathscr{F}} \notin \bigcup_{i=1}^m F_i$. By assumption, the net $x_{\mathscr{F}}$ has a cluster point x. Since $\mathscr{U}$ is a cover, we can find $U \in \mathscr{U}$ with $x \in U$. Since $x_{\mathscr{F}}$ is frequently in U we can find a finite subfamily $\mathscr{G} \in \mathfrak{S}$ so that $\{U\} \prec \mathscr{G}$ and $x_{\mathscr{G}} \in U$. Since $\{U\} \prec \mathscr{G}$, $U \subset \bigcup_{G \in \mathscr{G}} G$, and so $x_{\mathscr{G}} \in \bigcup_{G \in \mathscr{G}} G$, which is a contradiction.

Suppose that S is compact and let $\{y_\alpha\}_{\alpha \in I}$ be a net. If $\{y_\alpha\}$ has no cluster points, then for any $x \in S$, there is an open set U_x containing x and an $\alpha_x \in I$ with $y_\alpha \notin U_x$ if $\alpha \succ \alpha_x$. The family $\{U_x \mid x \in S\}$ is an open cover of S, so we can find $x_1, \ldots, x_n$ so that $\bigcup_{i=1}^n U_{x_i} = S$. Since I is directed, we can find $\alpha_0 \succ \alpha_{x_i}$ for $i = 1, \ldots, n$. But $y_{\alpha_0} \notin U_{x_i}$, $i = 1, \ldots, n$, which is impossible since $\bigcup_{i=1}^n U_{x_i} = S$. This contradiction establishes that $\{y_\alpha\}_{\alpha \in I}$ has a cluster point and thus a convergent subnet. ∎

Second countable spaces are compact if and only if every sequence has a convergent subsequence (this can be shown by mimicking the above proof).

Example 1 The unit ball in ℓ_2 is not compact in the *metric topology*. No subset of a sequence of orthonormal elements can converge.

Example 2 Let $S = \{\{a_n\} \in \ell_2 \mid |a_n| \leq 1/n\}$. It is easy to see that a sequence of elements of S converges if and only if each component converges. Using the diagonalization trick, we conclude that every sequence has a convergent subsequence. Therefore, by the Bolzano–Weierstrass theorem, S is compact.

Warning Compact is not the same as closed and bounded in a general Banach space. In fact the unit ball in a Banach space is compact (in the norm topology) if and only if the space is finite dimensional (see Problem 4 of Chapter V).

We now mention two simple "hereditary" properties of compact spaces (see Problem 38):

Proposition (a) A closed subset of a compact space is compact in the relative topology.

(b) A continuous image of a compact space is compact.

Corollary Any continuous function on a compact space takes on its maximum and minimum values. That is, there are $x_\pm$ so that

$$f(x_+) = \sup_{x \in C} f(x) \qquad \text{and} \qquad f(x_-) = \inf_{x \in C} f(x)$$

The following theorem is often useful:

Theorem IV.4 Let S and T be compact Hausdorff spaces; let $f: S \to T$ be a continuous bijection. Then f is a homeomorphism.

We need the following lemma:

Lemma If T is Hausdorff and $S \subset T$ is compact, then S is closed.

Proof. Let $x \in \bar{S}$. We can find a net $\{x_\alpha\}_{\alpha \in I}$ in S with $x_\alpha \to x$. Since limits are unique in Hausdorff spaces, x is the only cluster point of the net. But since S is compact, the net has a cluster point in S, that is, $x \in S$. Thus $S = \bar{S}$. ∎

Proof of Theorem IV.4 We need only prove f is open or equivalently, since f is a bijection, that $f[C]$ is closed if C is closed. But if $C \subset S$ is closed, then C is compact. By the last proposition, $f[C]$ is compact. The result now follows from the lemma. ∎

Proposition If $\{A_i\}_{i=1}^n$ is a family of compact sets, then $\bigtimes_{i=1}^n A_i$ with the product topology is compact.

Proof Let $\{x_\alpha\}_{\alpha \in I}$ be a net in $A = \bigtimes_{i=1}^n A_i$, $x_\alpha = \langle x_\alpha^1, x_\alpha^2, \ldots, x_\alpha^n \rangle$. Since A_1 is compact, we can find a subnet $\{x_{\alpha(i)}\}_{i \in D_1}$ so that $\{x_{\alpha(i)}^1\}$ converges to an $x_1 \in A_1$. By a finite induction, we can find a subnet $\{x_{\alpha(i)}\}_{i \in D_n}$ so that $x_{\alpha(i)}^j$ converges to an $x_j \in A_j$ for each j. Then $\{x_{\alpha(i)}\}$ converges in A to $x = \langle x_1, \ldots, x_n \rangle$, so A is compact by the Bolzano–Weierstrass criterion. ∎

This last proposition is not deep; what is deep is that it remains true for an arbitrary product of compact spaces:

Theorem IV.5 (Tychonoff's theorem) Let $\{A_\alpha\}_{\alpha \in I}$ be a collection of compact spaces. Then $\bigtimes_{\alpha \in I} A_\alpha$ is compact in the product (that is weak) topology.

Since this theorem has a mildly complicated proof well-treated in the textbook literature, we refer the reader to the references given in the Notes. Let us, however, make several comments. We first remark that it is this theorem that supports the feeling that the weak topology is the "natural" topology for $\bigtimes_\alpha A_\alpha$. Another a priori candidate, the "box topology," which is generated by sets of the form $\bigtimes_\alpha U_\alpha$, where each U_α is open in A_α is not a topology for

which Tychonoff's theorem holds. Secondly, we note that this theorem depends crucially on the axiom of choice (Zorn's lemma). In fact it is known that, set theoretically speaking, Tychonoff's theorem implies Zorn's lemma. Finally, we note that in the special case of countably many *metric* spaces, Theorem IV.5 can be proven by the method of the proposition and the diagonal trick of Section I.5.

Next, we would like to discuss functions on compact Hausdorff spaces. We first show that compact Hausdorff spaces have strong separation properties in the sense of separating closed sets with open sets. We then use these separation properties to construct continuous functions:

Theorem IV.6 Any compact Hausdorff space X is normal (T_4).

Proof We first prove X is regular (T_3). Let $p \in X$ and let $C \subset X$ be closed with $p \notin C$. Since X is Hausdorff, we can find, for any $y \in C$, open and disjoint sets, U_y and V_y, so that $y \in U_y$, and $p \in V_y$. The $\{U_y\}_{y \in C}$ cover C, which is compact. Thus $U_{y_1}, \ldots, U_{y_n}$ cover C. Let $U = \bigcup_{i=1}^{n} U_{y_i}$; $V = \bigcap_{i=1}^{n} V_{y_i}$. Then U and V are open and disjoint with $C \subset U$ and $p \in V$. This shows that X is regular. Now let C, D be closed and disjoint. By repeating the above argument with D replacing p and "since X is regular" replacing "since X is Hausdorff," we prove that X is normal. ∎

Normal spaces always have lots of continuous functions for:

Theorem IV.7 (Urysohn's lemma) Let C and D be closed disjoint sets in a normal space, X. Then, there is a continuous function from X to $\mathbb{R}$ with $0 \leq f(x) \leq 1$ for all x such that $f(x) = 0$ if $x \in C$ and $f(x) = 1$ if $x \in D$.

Sketch of proof Using the normality of X, one constructs by induction for each dyadic rational (that is, $r = k/2^n$, k, n integers, $0 \leq k \leq 2^n$) open sets, U_r, with $C \subset U_r \subset \overline{U}_r \subset U_s \subset \overline{U}_s \subset X \backslash D$ if $r < s$. One uses the U_r to define a function with $f(x) < r$ if and only if $x \in U_r$. f can be shown to be continuous. For details, see the references discussed in the notes. ∎

We will see below that one can prove even stronger function theoretic results (Theorem IV.11).

As a final result about the general properties of functions on X we will prove that certain families are dense in $C_{\mathbb{R}}(X)$, the family of all real-valued continuous functions on X. We first note that our proof in Section I.5 for $C[a, b]$ holds on any compact set:

Proof We show that if $f \in B$, then $|f| \in B$. The result then follows from the formulas: $f \vee g = \frac{1}{2}|f-g| + \frac{1}{2}(f+g)$, $f \wedge g = -[(-f) \vee (-g)]$. Without loss suppose that $\|f\|_\infty \leq 1$. By the classical Weierstrass theorem, we can find a sequence of polynomials $P_n(x)$ converging uniformly to $|x|$ on $[-1, 1]$, for example $|P_n(x) - |x|| < 1/n$ for all x in $[0, 1]$. Since $\|f\|_\infty \leq 1$, it follows that $\|P_n(f) - |f|\|_\infty < 1/n$, i.e. $|f| = \lim_{n\to\infty} P_n(f)$. Since B is an algebra with $1 \in B$, $P_n(f) \in B$. Since B is closed, $|f| \in B$. ∎

Finally, the full Stone–Weierstrass theorem is a consequence of Lemma 2 and the following theorem which is of some interest in itself:

Theorem IV.12 (Kakutani–Krein theorem) Let X be a compact Hausdorff space. Any lattice $\mathscr{L} \subset C_{\mathbb{R}}(X)$ which is a closed subspace containing 1 and which separates points is all of $C_{\mathbb{R}}(X)$.

Proof Let $h \in C_{\mathbb{R}}(X)$ and let ε be given. We seek $f \in \mathscr{L}$ with $\|h - f\| < \varepsilon$. Suppose we can show for any $x \in X$, there is $f_x \in \mathscr{L}$ with $f_x(x) = h(x)$ and $h \leq f_x + \varepsilon$. Then for each x, find U_x, an open neighborhood of x with $h(y) \geq f_x(y) - \varepsilon$ for all $y \in U_x$ (by the continuity of $h - f_x$). The U_x cover X so let $U_{x_1}, \ldots, U_{x_n}$ be a subcover. Then $f = f_{x_1} \wedge \cdots \wedge f_{x_m}$ obeys $f(y) + \varepsilon = \min_i\{f_{x_i}(y) + \varepsilon\} \geq h(y)$. Moreover, since any $y \in U_{x_i}$ for some i, $f(y) - \varepsilon \leq f_{x_i}(y) - \varepsilon \leq h(y)$. Thus $\|f - h\|_\infty < \varepsilon$.

It remains to find some f_x with the desired properties. Since $\mathscr{L}$ separates points and $1 \in \mathscr{L}$, for any x and y in X, we can find $f_{xy} \in \mathscr{L}$ with $f_{xy}(x) = h(x)$ and $f_{xy}(y) = h(y)$. For each y, we can find V_y, an open set about y with $f_{xy}(z) + \varepsilon \geq h(z)$ for $z \in V_y$. $V_{y_1}, \ldots, V_{y_n}$ will cover X for suitable $y_1, \ldots, y_n$. If we take $f_x = f_{xy_1} \vee \cdots \vee f_{xy_n}$, then $f_x(x) = h(x)$, and for any $z \in X$

$$f_x(z) + \varepsilon = \max_{i=1,\ldots,n} \{f_{xy_i}(z) + \varepsilon\} \geq h(z)$$

This completes the proof. ∎

IV.4 Measure theory on compact spaces †

In this section, we wish to discuss several aspects of measure theory which are special for compact spaces. In particular, we will see that the dual of $C(X)$ can be interpreted as a space of measures (the Riesz–Markov theorem). Since many of the measure-theoretic proofs are not enlightening, we will not prove all of the theorems.

† A supplement to this section begins on p. 353.

The first question that arises is what to pick as the σ-field of measurable sets. Let us begin with a minimal family. We clearly want to integrate continuous functions $f \in C(X)$. This might lead one to suspect that we want to allow all closed (and open) sets to be measurable but this is not necessary:

Definition A G_δ set is a set which is a countable intersection of open sets.

Proposition Let X be a compact Hausdorff space and let $f \in C_{\mathbb{R}}(X)$. Then $f^{-1}([a, \infty))$ is a compact G_δ set.

Proof $f^{-1}([a, \infty))$ is closed and thus compact. Since

$$f^{-1}([a, \infty)) = \bigcap_{n=1}^{\infty} f^{-1}((a - 1/n, \infty))$$

it is a G_δ. ∎

Thus, to integrate continuous functions, we need only have compact G_δ's in our σ-field.

Definition The σ-field generated by the compact G_δ's in a compact space X is called the family of **Baire sets**. The functions $f: X \to \mathbb{R}$ (or $\mathbb{C}$) measurable relative to this σ-field are called **Baire functions**. A measure on the Baire sets is called a **Baire measure** if in addition it is finite, that is $\mu(X) < \infty$.

As in the case of the finite intervals of the real line and Lebesgue measure:

Theorem IV. 13 If μ is a Baire measure, then $C(X) \subset L^p(X, d\mu)$ for all p and $C(X)$ is dense in $L^1(X, d\mu)$ or any L^p space for $p < \infty$ (but *not* L^∞ except in pathological cases where $C(X)$ is already all of L^∞!).

Despite the fact that Baire sets are all that are needed, the reader no doubt wants to repress G_δ's and consider all **Borel** sets, i.e. the σ-field generated by all open sets. The question of extending Baire measures to Borel measures, that is, measures on all Borel sets, is answered by the following remarks:

(1) Every Baire measure is automatically **regular**, that is,

$$\begin{aligned}\mu(Y) &= \inf\{\mu(O) \mid Y \subset O,\ O \text{ open and Baire}\} \\ &= \sup\{\mu(C) \mid C \subset Y,\ C \text{ compact and Baire}\}\end{aligned}$$

Theorem IV.8 Let $C(X)$ be the family of all continuous complex-valued functions on a compact Hausdorff space, X, endowed with the norm $\|f\|_\infty = \sup_{x \in X} |f(x)|$. Let $C_{\mathbb{R}}(X) = \{f \in C(X) \mid f \text{ is real-valued}\}$. Then $C(X)$ is a complex Banach space and $C_{\mathbb{R}}(X)$ is a real Banach space.

The density theorem we state generalizes a classical theorem of Weierstrass which says that any real-valued continuous function on [0, 1] is a uniform limit (on [0, 1]) of polynomials (see Problems 19 and 20). Note that $C_{\mathbb{R}}(X)$ has a natural multiplication given by $(fg)(x) = f(x)g(x)$. A **subalgebra** of $C_{\mathbb{R}}(X)$ is a subspace closed under multiplication:

Theorem IV.9 (Stone–Weierstrass theorem) Let B be a subalgebra of $C_{\mathbb{R}}(X)$ which is closed in $\|\cdot\|_\infty$. We say that B separates points if, given any $x, y \in X$, we can find $f \in B$ with $f(x) \neq f(y)$. If B separates points, then either $B = C_{\mathbb{R}}(X)$ or for some $x_0 \in X$, $B = \{f \in C_{\mathbb{R}}(X) \mid f(x_0) = 0\}$. If $1 \in B$, and B separates points, $B = C_{\mathbb{R}}(X)$.

We defer the instructive lattice-theoretic proof to an appendix.

The fact that we deal with $C_{\mathbb{R}}(X)$ and not $C(X)$ is crucial (see Problem 15), but, by adding an extra hypothesis we can easily extend Theorem IV.9 to the complex case.

Theorem IV.10 (complex Stone–Weierstrass theorem) Let B be a subalgebra of $C(X)$ with the property that if f is in B, then the complex conjugate, $\bar{f}$, is in B also. If B is closed and separates points, then $B = C(X)$ or $B = \{f \mid f(x) = 0\}$ for some fixed x.

The complex conjugate condition is crucial. For example, let D be the unit disc in the complex plane. The functions analytic in the interior of D, continuous on all of D, are a closed subalgebra of D containing 1 and separating points which is not $C(D)$. It is, however, not closed under complex conjugation.

As an example of how to use the Stone–Weierstrass theorem as well as an example of how several functional analytic theorems can combine in a very powerful way, we prove an extension theorem for functions in $C(Y)$ for $Y \subset X$ when X is compact and Y is closed. Actually, this theorem is true if X is merely normal (Problem 18):

Theorem IV.11 (Tietze extension theorem) Let X be a compact space and let $Y \subset X$ be closed. Let f be any continuous real-valued function on Y. Then there is an $\tilde{f} \in C_{\mathbb{R}}(X)$ so that $f(y) = \tilde{f}(y)$ for all $y \in Y$.

Proof Consider the map $\rho: C_{\mathbb{R}}(X) \to C_{\mathbb{R}}(Y)$ given by $\rho(f) = f \restriction Y$. The theorem is equivalent to the statement that ρ is onto. Clearly, Ran ρ is a subalgebra of $C_{\mathbb{R}}(Y)$ and $1 \in \text{Ran}\,\rho$. Moreover, by Urysohn's lemma, Ran ρ separates points. If we can show that Ran ρ is closed in $\|\cdot\|_{C(Y)}$ we can complete the proof by using the Stone–Weierstrass theorem.

Let $I = \text{Ker}\,\rho$. Then I is clearly closed in $C_{\mathbb{R}}(X)$, so we can form the quotient Banach space $C_{\mathbb{R}}(X)/I$. By elementary algebra, ρ "lifts" to a bijection, $\tilde{\rho}: C_{\mathbb{R}}(X)/I \to \text{Ran}\,\rho$. If we can prove $\|\tilde{\rho}([f])\|_{C_{\mathbb{R}}(Y)} = \|[f]\|_{C_{\mathbb{R}}(X)/I}$, Ran ρ will be a Banach space and thus closed.

Clearly, $\|\rho(f)\|_{C_{\mathbb{R}}(Y)} \leq \|f\|_{C_{\mathbb{R}}(X)}$, so $\|\tilde{\rho}([f])\|_{C_{\mathbb{R}}(Y)} \leq \|[f]\|_{C_{\mathbb{R}}(X)/I}$. Thus, it is enough to show that given $g \in \text{Ran}\,\rho$, we can find $f \in C_{\mathbb{R}}(X)$ with $g = \rho(f)$ and $\|g\|_{C_{\mathbb{R}}(Y)} = \|f\|_{C_{\mathbb{R}}(X)}$ (remember the definition of quotient norm!). Since $g \in \text{Ran}\,\rho$, we know that $g = \rho(h_1)$ for some $h_1 \in C_{\mathbb{R}}(X)$. Let

$$h_2 = \min\{\|g\|_{C_{\mathbb{R}}(Y)}, h_1\}$$

so that $\rho(h_2) = g$ and $h_2(x) \leq \|g\|_{C_{\mathbb{R}}(Y)}$ for all x. Let $h_3 = \max\{-\|g\|_{C_{\mathbb{R}}(X)}, h_2\}$. Then, $\|h_3\|_{C_{\mathbb{R}}(X)} = \|g\|_{C_{\mathbb{R}}(Y)}$ and $\rho(h_3) = g$. This completes the proof. ∎

Appendix to IV.3 The Stone–Weierstrass theorem

In this appendix we prove Theorem IV.9 in the case $1 \in B$. The general proof is left as an exercise. Interestingly enough, the first step in the proof is the proof of the classical Weierstrass theorem (which is a special case of the general theorem!)

Lemma 1 The polynomials are dense in $C_{\mathbb{R}}[a, b]$ for any finite real numbers a, b.

Proof See Problems 19 and 20.

This can now be used to prove that B is a lattice, where:

Definition A subset $S \subset C_{\mathbb{R}}(X)$ is called a lattice if for all $f, g \in S$, $f \wedge g = \min\{f, g\}$ and $f \vee g = \max\{f, g\}$ are in S.

Lemma 2 Any closed subalgebra B of $C_{\mathbb{R}}(X)$ with $1 \in B$ is a lattice.

Theorem IV.15 (monotone convergence theorem for nets) Let μ be a regular Borel measure on a compact Hausdorff space X. Let $\{f_\alpha\}_{\alpha\in I}$ be an increasing net of continuous functions. Then $f = \lim_\alpha f_\alpha \in L^1(X, d\mu)$ if and only if $\sup_\alpha \|f_\alpha\|_1 < \infty$ and in that case $\lim_\alpha \|f - f_\alpha\|_1 = 0$.

Before leaving measure theory on compact spaces, we should identify the dual space of $C(X)$. Of course, not every continuous linear functional on $C(X)$ is a positive linear functional, but the major result we are heading toward is that any $\ell \in C_{\mathbb{R}}(X)^*$ is the difference of two positive linear functionals. This depends on a simple "lattice-theoretic" result about $C_{\mathbb{R}}(X)$:

Lemma Let $f, g \in C_{\mathbb{R}}(X)$ with $f, g \geq 0$. Suppose $h \in C_{\mathbb{R}}(X)$ and $0 \leq h \leq f + g$. Then, we can write $h = h_1 + h_2$ with $0 \leq h_1 \leq f$, $0 \leq h_2 \leq g$, $h_1, h_2 \in C_{\mathbb{R}}(X)$.

Proof Let $h_1 = \min\{f, h\}$. Then $0 \leq h_1 \leq f$ and if $h_2 \equiv h - h_1$, then $h_2 \geq 0$. Moreover, if $h_1(x) = h(x)$, then $h_2(x) = 0 \leq g(x)$ and if $h_1(x) = f(x)$, then $h_2(x) = h(x) - f(x) \leq f(x) + g(x) - f(x) = g(x)$, so $h_2 \leq g$. ∎

Theorem IV.16 Let $\ell \in C_{\mathbb{R}}(X)^*$. Then ℓ can be written $\ell = \ell_+ - \ell_-$ with ℓ_+ and ℓ_- positive linear functionals. Moreover, $\ell_+(1) + \ell_-(1) = \|\ell\|$ and this uniquely determines ℓ_+ and ℓ_-.

Proof For $f \in C(X)_+ \equiv \{f \in C(X) \mid f \geq 0\}$, define $\ell_+(f) = \sup\{\ell(h) \mid h \in C(X); 0 \leq h \leq f\}$. Since $|\ell(h)| \leq \|\ell\| \, \|h\|_\infty \leq \|\ell\| \, \|f\|_\infty$, this supremum is finite. Clearly $\ell_+(tf) = t\ell_+(f)$ for any scalar $t > 0$ and $\ell_+(f) \geq \ell(0) = 0$ for all $f \in C(X)_+$. Let $f, g \in C(X)_+$. Then, by the lemma:

$$\begin{aligned}\ell_+(f+g) &= \sup\{\ell(h) \mid 0 \leq h \leq f+g\} \\ &= \sup\{\ell(h_1) + \ell(h_2) \mid 0 \leq h_1 \leq f, \quad 0 \leq h_2 \leq g\} \\ &= \ell_+(f) + \ell_+(g)\end{aligned}$$

For any $f \in C(X)$, define $f_+ = \max\{f, 0\}$ and $f_- = -\min\{f, 0\}$, so $f = f_+ - f_-$. Define $\ell_+(f) = \ell_+(f_+) - \ell_+(f_-)$. It is then easy to show ℓ_+ is linear on $C(X)$. By definition $\ell_+(f) \geq \ell(f)$ if $f \geq 0$ so $\ell_-(f) \equiv \ell_+(f) - \ell(f)$ is a positive linear functional. We have thus written $\ell = \ell_+ - \ell_-$ as the difference of positive linear functionals.

To prove $\ell_+(1) + \ell_-(1) = \|\ell\|$, we note first $\|\ell\| \leq \|\ell_+\| + \|\ell_-\| = \ell_+(1) + \ell_-(1)$. For the inequality in the other direction, we first rewrite ℓ_- in a way symmetric to ℓ_+. For $f \geq 0$

$$\begin{aligned}\ell_-(f) &= \sup\{\ell(h) - \ell(f) \mid 0 \leq h \leq f\} \\ &= \sup\{\ell(k) \mid -f \leq k \leq 0\}\end{aligned}$$

where $k = h - f$. Thus:

$$\begin{aligned}\ell_+(1) + \ell_-(1) &= \sup\{\ell(h) \mid 0 \le h \le 1\} + \sup\{\ell(k) \mid -1 \le k \le 0\} \\ &= \sup\{\ell(g) \mid -1 \le g \le 1\} \\ &\le \|\ell\| \sup\{\|g\|_\infty \mid -1 \le g \le 1\} \\ &= \|\ell\|\end{aligned}$$

The proof of uniqueness is left to the reader (Problem 31). ∎

Definition A **complex Baire measure** is a finite linear complex combination of Baire measures.

An easy consequence of Theorem IV.14 and Theorem IV.16 is:

Theorem IV.17 Let X be a compact space. Then the dual $C(X)^*$ of $C(X)$ is the space of all complex Baire measures.

Definition We write $\mathcal{M}(X) = C(X)^*$; $\mathcal{M}_+(X) = \{\ell \in \mathcal{M}(X) \mid \ell$ is a positive linear functional$\}$ and $\mathcal{M}_{+,1}(X) = \{\ell \in \mathcal{M}_+ \mid \|\ell\| = 1\}$.

In some cases, it is important to think of measures not merely as individual objects but instead as elements of $\mathcal{M}(X)$, so that we can employ geometric ideas. To give the reader a feel for this sort of reasoning we conclude our discussion of $\mathcal{M}(X)$ by a simple convexity theorem.

Definition A set A in a vector space Y is called **convex** if x and $y \in A$ and $0 \le t \le 1$ implies $tx + (1 - t)y \in A$. Thus A is convex if the line segment between x and y is in A whenever x and y are in A (Figure IV.1). A is called a **cone** if $x \in A$ implies $tx \in A$ for all $t > 0$. If A is convex and a cone, it is called a **convex cone.**

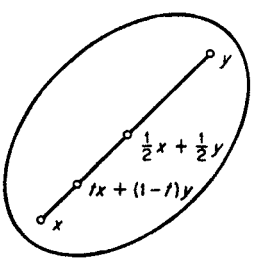

FIGURE IV.1 A convex set.

(2) In general, a Baire measure has many extensions to all Borel sets but there is exactly one regular extension to a Borel measure. A Borel measure is called regular if

$$\begin{aligned}\mu(Y) &= \inf\{\mu(O) \mid Y \subset O,\ O \text{ open}\} \\ &= \sup\{\mu(C) \mid C \subset O,\ C \text{ compact and } \textit{Borel}\}\end{aligned}$$

Thus there is a one-one correspondence between Baire measures and *regular* Borel measures.

(3) If μ is a Borel measure, then $C(X)$ is dense in $L^1(X, d\mu)$ if and only if μ is regular. If μ is regular, every Borel set is almost everywhere a Baire set in the sense that given a Borel set Y, there is a a Baire set $\tilde{Y}$ with

$$\int |\chi_Y - \chi_{\tilde{Y}}|\, d\mu \equiv \mu(Y \backslash \tilde{Y}) + \mu(\tilde{Y} \backslash Y) = 0$$

In addition, every Borel function is equal, after a change on a Borel set of measure zero, to a Baire function.

(4) In certain cases, every compact set is a G_δ, so the Baire and Borel sets are identical. This is the case if X is a compact metric space (see Problem 30).

Henceforth, we will use the word measure in the context of a compact set, X, to mean Baire (or equivalently regular Borel) measure unless we specifically indicate otherwise.

Now, let X be compact and let μ be a measure on X. Consider the map $C(X) \to \mathbb{C}$ given by $f \mapsto \ell_\mu(f) \equiv \int f\, d\mu$. ℓ_μ is clearly linear and

$$|\ell_\mu(f)| \leq \int |f|\, d\mu \leq \|f\|_\infty \mu(X)$$

so ℓ_μ is a continuous linear functional on $C(X)$. In fact, $\|\ell_\mu\|_{C(X)^*} \equiv \mu(X)$, for take $f = 1$. Moreover, ℓ_μ is positive in the sense:

Definition A **positive linear functional** on $C(X)$ is a (not necessarily a priori continuous) linear functional ℓ with $\ell(f) \geq 0$ for all f with $f \geq 0$ pointwise.

In the more general context of C^*-algebras, positive linear functionals will again arise; see Chapter XVII. They have the following nice property (for other properties of positivity, see Problem 37):

Proposition Let ℓ be a positive linear functional. Then ℓ is continuous and $\|\ell\|_{C(X)^*} = \ell(1)$.

Proof Suppose first that f is real. Since $-\|f\|_\infty \le f \le \|f\|_\infty$, we have $-\ell(1)\|f\|_\infty \le \ell(f) \le \ell(1)\|f\|_\infty$; that is, $|\ell(f)| \le \|f\|_\infty \ell(1)$. If f is arbitrary, $\ell(f) = e^{i\phi}r$ with r real and positive, so

$$|\ell(f)| = \ell(\mathrm{Re}[e^{-i\phi}f]) \le \|\mathrm{Re}(e^{-i\phi}f)\|_\infty \ell(1) \le \ell(1)\|f\|_\infty \quad \blacksquare$$

We have seen that any Baire measure provides an example of a positive linear functional on $C(X)$; that these are the only examples is the content of:

Theorem IV.14 (the Riesz–Markov theorem) Let X be a compact Hausdorff space. For any positive linear functional ℓ on $C(X)$ there is a unique Baire measure μ on X with

$$\ell(f) = \int f d\mu$$

While we will not give a detailed proof, let us show how μ may be recovered from ℓ_μ. A similar process allows one to construct a measure from any positive linear functional, even if one does not know a priori that it is of the form ℓ_μ. Since μ is inner regular (that is, $\mu(Y) = \sup\{\mu(C) \mid C \subset Y, C \text{ compact}\}$), we need only find $\mu(C)$ for C compact to "recover" μ. We claim $\mu(C) = \inf\{\ell_\mu(f) \mid f \in C(X), f \ge \chi_C\}$. Since μ is positive, it is clear that $\mu(C) \le \ell_\mu(f)$ if $f \ge \chi_C$; thus, we need only show that, given ε, we can find $f \in C(X)$ with $\chi_C \le f$ and $\ell_\mu(f) \le \mu(C) + \varepsilon$. Since μ is outer regular, given ε we can find O open with $\mu(O \backslash C) < \varepsilon$ and $C \subset O$. By Urysohn's lemma, we can find $f \in C(X)$ with $0 \le f \le 1$, $f(x) = 1$ if $x \in C$ and $f(x) = 0$ if $x \in X \backslash O$. Thus $\ell(f) \le \mu(O) < \mu(C) + \varepsilon$. This shows μ can be recovered from ℓ_μ, and so it is not too surprising that a measure can be constructed from an arbitrary ℓ.

The Riesz-Markov theorem is the usual way that measures arise in functional analysis. For example, we have already intimated that measures on $\mathbb{R}$ are associated with quantum mechanical Hamiltonians and they, in turn, arise from certain positive linear functions and the use of the Riesz–Markov theorem (or rather its extension to locally compact spaces which we will discuss shortly).

In general, a pointwise limit of a net of Baire functions is not a Baire or even a Borel function (Problem 13). However, if $\{f_\alpha\}_{\alpha \in I}$ is a net of functions with each f_α continuous and $\{f_\alpha\}$ is increasing in the sense that $f_\alpha \ge f_\beta$ if $\alpha \succ \beta$, then $f = \lim_\alpha f_\alpha = \sup_\alpha f_\alpha$ is a Borel function because

$$f^{-1}[(a, \infty)] = \bigcup_\alpha f_\alpha^{-1}[(a, \infty)]$$

is open. The monotone convergence theorem has the following net generalization:

Proposition Let X be a compact Hausdorff space. Then $\mathcal{M}_{+,1}(X)$ is convex and $\mathcal{M}_{+}(X)$ is a convex cone.

Proof A convex combination of positive linear functionals is clearly a positive linear functional. Moreover, $\|\ell\| = \ell(1)$ if ℓ is a positive linear functional so $\|t\ell_1 + (1-t)\ell_2\| = 1$, if $\ell_1, \ell_2 \in \mathcal{M}_{+,1}$. ∎

At first sight, this geometric fact may appear a little strange since the reader is used to thinking of the unit sphere, $\{x \mid \|x\| = 1\}$ as "round" and here we are saying a piece of it is absolutely flat! The moral is that every norm is not the Euclidean norm (the parallelogram law implies that in a Hilbert space, if $\|x\| = \|y\| = 1$, and $x \neq y$, then $\|tx + (1-t)y\| < 1$). In fact, $\mathbb{R}^n$ with the norm $\|\langle x_1, \ldots, x_n\rangle\| = \sum_{i=1}^{n} |x_i|$ has a unit sphere with flat faces, see Figure IV.2. This is not a coincidence; $\{1, \ldots, n\}$ is a compact set when given the discrete topology, and $\mathbb{R}^n$ with the norm considered is precisely $\mathcal{M}(\{1, \ldots, n\})$.

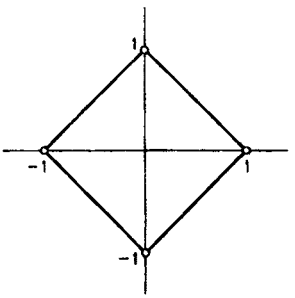

FIGURE IV.2 The unit sphere in R^2 when $\|\langle x, y\rangle\| = |x| + |y|$.

Now, we want to extend "topological measure theory" to a larger class of spaces:

Definition A topological space, X is called **locally compact** if and only if every point $p \in X$, has a compact neighborhood.

By thinking of Lebesgue measure on $\mathbb{R}$, we realize that we want to relax the condition $\mu(X) < \infty$ which we required when X was compact. We first define the Baire sets in X, a locally compact space, to be the σ-ring $\mathcal{B}$ generated by compact G_δ sets. Note that, in general, X may not be a set of $\mathcal{B}$. However, if X is σ-compact, that is, a countable union of compact sets, X is in $\mathcal{B}$.

Definition A **Baire measure** on X, a locally compact space, is a measure on the Baire sets for which $\mu(C) < \infty$ for any compact Baire set C.

Given any Baire measure μ on X, and given a compact G_δ set $C \subset X$, there is induced by restriction a Baire measure μ_C on C. Conversely, it is easy to see that a family of measures $\{\mu_C\}$, one for each compact G_δ set, with the property that $\mu_C(Y) = \mu_D(Y)$ if $Y \subset C \cap D$, defines a Baire measure. This association allows us to prove theorems in the locally compact case from their compact case analogues.

Definition Let X be a locally compact space. $\kappa(X)$, the algebra of **continuous functions of compact support,** is the set of functions that vanish outside some compact set. $C_\infty(X)$, the algebra of continuous functions vanishing at ∞, is the set of $f \in C(X)$ with the property that for any $\varepsilon > 0$, there is a compact set $D_\varepsilon \subset X$ such that $|f(x)| < \varepsilon$ if $x \notin D_\varepsilon$. Thus

$$\kappa(X) \subset C_\infty(X) \subset C(X)$$

With this definition, Theorem IV.14 implies

Theorem IV. 18 (Riesz–Markov) Let X be a locally compact space. A positive linear functional on $\kappa(X)$ is of the form $\ell(f) = \int f \, d\mu$ for some Baire measure, μ. A positive linear functional on $C_\infty(X)$ comes from a measure μ with total finite mass, that is, $\sup_{A \in \mathcal{B}} \mu(A) < \infty$.

In the next chapter, we will find a topology on $\kappa(X)$ for which the dual is just the complex Baire measures. Notice that this topology is *not* given by $\|\cdot\|_\infty$. $\kappa(X)$ is not complete in the norm $\|\cdot\|_\infty$; its completion is $C_\infty(X)$ and its dual in $\|\cdot\|_\infty$ is the *finite* measures.

IV.5 Weak topologies on Banach spaces †

Definition Let X be a Banach space with dual space X^*. The **weak topology on** X is the weakest topology on X in which each functional ℓ in X^* is continuous.

Thus a neighborhood base at zero for the weak topology is given by the sets of the form

$$N(\ell_1, \ldots, \ell_n; \varepsilon) = \{x \mid |\ell_i(x)| < \varepsilon; \quad i = 1, \ldots, n\}$$

† A supplement to this section begins on p. 354.

that is, neighborhoods of zero contain cylinders with finite-dimensional open bases. A net $\{x_\alpha\}$ converges weakly to x, written $x_\alpha \xrightarrow{w} x$, if and only if $\ell(x_\alpha) \to \ell(x)$ for all $\ell \in X^*$.

For infinite dimensional Banach spaces, the weak topology does not arise from a metric. This is one of the main reasons we have introduced topological spaces. Before considering examples, let us note three elementary properties of the weak topology:

Proposition (a) The weak topology is weaker than the norm topology, that is, every weakly open set is norm open.

(b) Every weakly convergent *sequence* is norm bounded.

(c) The weak topology is a Hausdorff topology.

Proof (a) follows from $|\ell(x)| \leq \|\ell\| \, \|x\|$; (b) is a consequence of the uniform boundedness principle; and (c) follows from the Hahn–Banach theorem. We leave the details to the reader. ∎

We emphasize that (b) is only true for sequences. In Problem 39, the reader is asked to construct a counterexample to the analogous net statement.

Let us consider two examples; in both of them, we will describe what it means for sequences to converge. This does *not* completely describe the topology, but it will give the reader an impressionistic view of the underlying topology.

Example 1 Let $\mathscr{H}$ be a Hilbert space. Let $\{\varphi_\alpha\}_{\alpha \in I}$ be an orthonormal basis for $\mathscr{H}$. Given a *sequence* $\psi_n \in \mathscr{H}$, let $\psi_n^{(\alpha)} = \langle \varphi_\alpha, \psi_n \rangle$ be the coordinates of ψ_n. We claim $\psi_n \to \psi$ in the weak topology if and only if (a) $\psi_n^{(\alpha)} \to \psi^{(\alpha)}$ for each α and (b) $\|\psi_n\|$ is bounded. For suppose $\psi_n \xrightarrow{w} \psi$; then (a) follows by definition and (b) comes from (ii) of the proposition. On the other hand, let (a) and (b) hold and let $F \subset \mathscr{H}$ be the subspace of finite linear combinations of the φ_α. By (a), $\langle \varphi, \psi_n \rangle \to \langle \varphi, \psi \rangle$ if $\varphi \in F$. Using the fact that X is dense, (b), and an $\varepsilon/3$ argument, the weak convergence follows.

Example 2 Let X be a compact Hausdorff space and consider the weak topology on $C(X)$. Let $\{f_n\}$ be a sequence in $C(X)$. We claim $f_n \to f$ in the weak topology if and only if (a) $f_n(x) \to f(x)$ for each $x \in X$, and (b) $\|f_n\|$ is bounded. For if $f_n \xrightarrow{w} f$, then (a) holds since $f \mapsto f(x)$ is an element of $C(X)^*$ and (b) comes from (ii) of the proposition. On the other hand, if (a) and (b) hold, then $|f_n(x)| \leq \sup_n \|f_n\|_\infty$ which is L^1 with respect to any Baire measure μ.

Thus, by the dominated convergence theorem, for any $\mu \in \mathcal{M}_+(X)$, $\int f_n \, d\mu \to \int f \, d\mu$. Since any $\ell \in \mathcal{M}(X)$ is a finite linear combination of measures in $\mathcal{M}_+$, we conclude that $f_n \to f$ weakly.

We have seen that the weak topology is weaker than the norm topology; actually, it is very weak indeed! To see this, we note that having few open sets is the same as having few closed sets and this is the same as big closures. In Problem 40, the reader will prove that the weak closure of the unit sphere, $\{x \in X \mid \|x\| = 1\}$, in X is the unit ball, $\{x \mid \|x\| \leq 1\}$, in any infinite dimensional Banach space.

We will shortly study general "dual" topologies. As a special case of Theorem IV.20, we state;

Theorem IV.19 A linear functional ℓ on a Banach space is weakly continuous if and only if it is norm continuous.

While this theorem follows from Theorem IV.20, it has a simple direct proof (Problem 42).

Finally, we should like to discuss the weak-* topology and prove a compactness theorem which will often be of use to us. Suppose $Y = X^*$ is the dual of some Banach space X. $Y^* = X^{**}$, of course, induces the weak topology on Y, but we may instead consider the topology induced by X acting on X^*; explicitly:

Definition Let X^* be the dual of a Banach space. The **weak-* topology** is the weakest topology on X^* in which all the functions $\ell \mapsto \ell(x)$, $x \in X$, are continuous.

Notice that the weak-* topology is even weaker than the weak topology. As one might expect, X is reflexive if and only if the weak and weak-* topologies coincide, and many characterizations of reflexivity depend on relations involving the weak and weak-* topologies.

To avoid confusion and to be able to state our next theorem in its natural setting, let us introduce a new notion:

Definition Let X be a vector space and let Y be a family of linear functionals on X which separates points of X. Then the **Y-weak topology on X**, written $\sigma(X, Y)$, is the weakest topology on X for which all the functionals in Y are continuous.

Because Y is assumed to separate points, $\sigma(X, Y)$ is a Hausdorff topology on X. For example, the weak topology on X is the $\sigma(X, X^*)$ topology while the $\sigma(X^*, X)$ topology is the weak-* topology on X^*. The $\sigma(X, Y)$ topology depends only on the vector space generated by Y, so we henceforth suppose that Y is a vector space.

Example The weak-* topology on $\mathcal{M}(X)$, X a compact Hausdorff space, is often called the **vague** topology. To get an idea of how weak it is, let us show the linear combinations of point masses are weak-* dense in $\mathcal{M}(X)$. In Problem 41, the reader is asked to show they are actually norm closed. Suppose that μ is a given measure. We must show that every weak neighborhood of μ contains a sum of point measures, or equivalently, given $f_1, \ldots, f_n$ and ε, that we can find $\alpha_1, \ldots, \alpha_m$ and $x_1, \ldots, x_m$ so that

$$|\mu(f_i) - \sum_{j=1}^{m} \alpha_j f_i(x_j)| < \varepsilon \qquad \text{for} \quad i = 1, \ldots, n$$

For then $\sum \alpha_j \delta_{x_j}$ will be in the vague neighborhood $N(f_1, \ldots, f_n, \varepsilon) + \mu$. Without loss, suppose that $f_1, \ldots, f_n$ are linearly independent. For each x, consider the vector $\mathbf{f}_x = \langle f_1(x), \ldots, f_n(x) \rangle \in \mathbb{R}^n$. If the $\{\mathbf{f}_x\}$ do not span $\mathbb{R}^n$ there is an $\mathbf{a} = \langle a_1, \ldots, a_n \rangle \neq 0 \in \mathbb{R}^n$ with $\mathbf{a} \cdot \mathbf{f}_x = 0$ for all x, that is, $\sum_{i=1}^{n} a_i f_i = 0$ contradicting linear independence. Thus, the $\mathbf{f}_x$ span $\mathbb{R}^n$. So, we can find $x_1, \ldots, x_n$ and $\alpha_1, \ldots, \alpha_n$ with

$$\langle \mu(f_1), \ldots, \mu(f_n) \rangle = \sum_{i=1}^{n} \alpha_i \mathbf{f}_{x_i}$$

So, $\mu(f_i) = \sum_{j=1}^{n} \alpha_j f_i(x_j)$, which proves our claim.

The $\sigma(X^*, X)$ topology is of course weaker than the norm topology on X^* so all the $\sigma(X^*, X)$-continuous linear functionals are in X^{**}. In general, however, not all of X^{**} is weak-* continuous on X^*; in fact:

Theorem IV.20 The $\sigma(X, Y)$ continuous linear functionals on X are precisely Y; in particular the only weak-* continuous functionals on X^* are the elements of X.

Proof Suppose that ℓ is a $\sigma(X, Y)$ continuous functional on X. Then $\{x \mid |\ell(x)| < 1\} \supset \{x \mid |y_i(x)| < \varepsilon;\ i = 1, \ldots, n\}$ for some ε and some $y_1, \ldots, y_n \in Y$. Now suppose that $y_i(x) = 0$ for $i = 1, \ldots, n$. Then $|\ell(\varepsilon^{-1}x)| < 1$ for all $\varepsilon > 0$, which implies that $\ell(x) = 0$. As a result, ℓ lifts to a functional $\tilde{\ell}$ on X/K where $K = \{x \mid y_i(x) = 0, i = 1, \ldots, n\}$. Elementary abstract algebra shows $\tilde{y}_1, \ldots, \tilde{y}_n$ span the dual space of X/K. Thus $\tilde{\ell} = \sum_{i=1}^{n} \alpha_i \tilde{y}_i$, so that $\ell = \sum_{i=1}^{n} \alpha_i y_i \in Y$. ∎

Finally, we conclude this section with its most important result, a result which is perhaps the most important consequence of Tychonoff's theorem:

Theorem IV. 21 (the Banach–Alaoglu theorem) Let X^* be the dual of some Banach space, X. Then the unit ball in X^* is compact in the weak-$*$ topology.

Proof For each $x \in X$, let $B_x = \{\lambda \in \mathbb{C} \mid |\lambda| \leq \|x\|\}$. Each B_x is compact, so, by Tychonoff's theorem, $B = \bigtimes_{x \in X} B_x$ is compact in the product topology. Now what is B? An element of B is just an assignment of a number $b(x) \in B_x$ for each x in X, that is, b is a function from X to $\mathbb{C}$ with $|b(x)| \leq \|x\|$. In particular, the unit ball $(X^*)_1$ is a subset of B, namely those $b \in B$ which are linear. What is the relative topology induced on $(X^*)_1$ by the product topology on B? It is precisely the weakest topology making $\ell \mapsto \ell(x)$ continuous for each x, that is, the weak-$*$ topology.

Thus, we must only show that $(X^*)_1$ is closed in the product topology. Suppose that ℓ_α is a net in $(X^*)_1$ with $\ell_\alpha \to \ell$. Since $|\ell(x)| \leq \|x\|$, we need only show ℓ is linear. But this is easy; if $x, y \in X$ and $\lambda, \mu \in \mathbb{C}$, then

$$\ell(\lambda x + \mu y) = \lim_\alpha \ell_\alpha(\lambda x + \mu y) = \lim_\alpha \lambda \ell_\alpha(x) + \mu \ell_\alpha(y)$$

$$= \lambda \ell(x) + \mu \ell(y) \quad \blacksquare$$

Appendix to IV.5 Weak and strong measurability

In Section II.1, we briefly discussed vector-valued measurable functions with values in an infinite dimensional Hilbert space $\mathscr{H}$. f was called measurable (in Problem 12 of Chapter II) if $(y, f(\cdot))$ was a complex-valued measurable function for each $y \in \mathscr{H}$. This notion might be called **weak measurability**. Another natural candidate for measurability is the a priori stronger notion of measurability which requires that $f^{-1}[C]$ be measurable for each open set $C \subset \mathscr{H}$. *Throughout this book, by a vector-valued measurable function, we will mean a function measurable in the weak sense.* However, to satisfy the reader's natural curiosity, a brief comparison of the various notions of measurability of vector-valued functions seems in order.

Definition Let f be a function on a measure space $\langle M, \mu, \mathscr{R} \rangle$ taking values in a Banach space E.

(i) f is called **strongly measurable** if and only if there is a sequence of functions f_n so that $f_n(x) \to f(x)$ in norm for a.e. $x \in M$ and each f_n takes only finitely many values, each value being taken on a set in $\mathscr{R}$.

(ii) f is called **Borel measurable** if $f^{-1}[C] \in \mathscr{R}$ for each open set C in E (in the metric space topology on E).

(iii) f is called **weakly measurable** if and only if $\ell(f(x))$ is a complex-valued measurable function for each $\ell \in E^*$.

Proposition (a) A pointwise limit of a sequence of Borel measurable functions is a Borel measurable function.

(b) Let f be a function from M to E. If f is strongly measurable, then f is Borel measurable.

(c) Let f be a function from M to E. If f is Borel measurable, it is weakly measurable.

Proof (a) Let $f_n \to f$ pointwise in norm. Let C be an open set in E. Let $C_k = \{x \mid B_{k^{-1}}^x \subset C\}$ where B_ε^x is the ball of radius ε about x. Then,

$$f^{-1}[C] = \bigcup_{k=1}^{\infty} \bigcup_{n=1}^{\infty} \bigcap_{m>n} f^{-1}[C_k]$$

so f is Borel measurable.

(b) This is a direct consequence of (a) and the definitions.

(c) The composition of Borel functions is Borel. ∎

Theorem IV.22 Let $\mathscr{H}$ be a separable Hilbert space. Let f be a function from a measure space $\langle M, \mu, \mathscr{R} \rangle$ to $\mathscr{H}$. Then the following three statements are equivalent:

(a) f is strongly measurable.
(b) f is Borel measurable.
(c) f is weakly measurable.

Proof By the last proposition, we need only show that (c) implies (a). Let $\{\psi_n\}_{n=1}^{\infty}$ be an orthonormal basis for $\mathscr{H}$. Let $a_n = (\psi_n, f(x))$. Each a_n is a complex-valued measurable function. It is easy to construct $a_{n,m}(x)$ finite valued, $|a_{n,m}(x)| < |a_n(x)|$ for all x and $\lim_{m\to\infty} a_{n,m}(x) = a_n(x)$ for all $x \in X$. Define $f_N = \sum_{n=1}^{N} a_{n,N}(x)\psi_n$. f_N is finite valued and $f_N \to f$ in norm so f is strongly measurable. ∎

Example Let $\mathbb{C}_t$ be a copy of the complex numbers $\mathbb{C}$ and let $\mathscr{H} = \oplus_{t\in\mathbb{R}} \mathbb{C}_t$, that is, $\mathscr{H}$ consists of functions φ on $\mathbb{R}$, nonzero at only count-

ably many t with $\sum_{t\in\mathbb{R}} |\varphi(t)|^2 < \infty$. Let φ_s be given by

$$\varphi_s(t) = \begin{cases} 1 & \text{if } t = s \\ 0 & \text{otherwise} \end{cases}$$

Then $\{\varphi_s\}_{s\in\mathbb{R}}$ is an orthonormal basis for $\mathscr{H}$. Let $f\colon \mathbb{R} \to \mathscr{H}$ be defined by $f(s) = \varphi_s$. For any $\psi \in \mathscr{H}$, $(\psi, f(s)) = 0$ except for a countable set so $(\psi, f(s))$ is measurable. Thus $f(s)$ is weakly measurable. But f is not strongly measurable; for if $f = \lim f_n$ pointwise in norm, then $\operatorname{Ran} f \in \overline{\bigcup \operatorname{Ran} f_n}$. If each f_n were finite valued, $\operatorname{Ran} f$ would be separable, which it is not.

NOTES

Section IV.1 For the reader who wishes to delve further into the realm of general point set topology, we recommend J. Kelley's *General Topology*, Van Nostrand–Reinhold, Princeton, New Jersey, 1955, most enthusiastically. The best way to read the book is to do all the problems; it is time consuming but well worth the effort if the reader can afford the time. Other good references on elementary (and sophisticated) topological notions include: K. Kuratowski, *Topology*, Vol. I, Academic Press, New York, 1966, W. Pervin, *Foundations of General Topology*, Academic Press, New York, 1964, and W. Thron, *Topological Structures*, Holt, New York, 1966.

The notion of topological spaces grew out of work of Fréchet and Hausdorff. The T_1–T_4 classification is due to P. Alexandroff and H. Hopf, in *Topologie I*, Berlin, 1935.

The concept of "Cauchy sequence" does not extend to an arbitrary topological space. However, one can add a "uniform structure" to the topological structure and thereby have spaces in which Cauchy sequence and completeness make sense. One thinks of neighborhoods of x as describing closeness to x. To have a notion of "closeness to x" uniform in x, we need a family $\mathscr{U}$ of subsets of $X \times X$ each containing the set $\Delta = \{\langle x, x\rangle \mid x \in X\}$. We need enough conditions on $\mathscr{U}$ so that $\mathscr{U}_x = \{U_x \mid U \in \mathscr{U}\}$ with $U_x = \{y \mid \langle x, y\rangle \in U\}$ is a neighborhood system for a topology. The canonical example is to let $\mathscr{U}$ be the family of all sets in $X \times X$ containing a set of the form $\{\langle x, y\rangle \mid \rho(x, y) < \varepsilon\}$ with ρ a metric. If G is a topological group (in particular, if G is a topological vector space), there is also a natural uniform structure given by $\mathscr{U} = \{U_N \mid N \in \eta\}$ where η the family of neighborhoods of the identity and $U_N = \{\langle x, y\rangle \mid xy^{-1} \in N\}$. Given a uniform structure $\mathscr{U}$, a net $\{x_\alpha \mid \alpha \in D\}$ is called a Cauchy net if and only if for each $U \in \mathscr{U}$, there is an $\alpha_0 \in D$ so that $\alpha, \beta > \alpha_0$ implies $\langle x_\alpha, x_\beta\rangle \in U$.

The notion of uniform space was first formalized in A. Weil, "Sur les espaces à structure uniforme et sur la topologie générale," *Actualités Sci. Ind.* **551**, Paris (1937). For a modern treatment of uniform spaces, see Kelley, Chapter 6, or G. Choquet, *Lectures on Analysis*, Benjamin, New York, §5.

Section IV.2 Nets were first introduced in E. H. Moore and H. L. Smith, "A General Theory of Limits," *Amer. J. Math.* **44** (1922), 102, and the theory is sometimes called Moore–Smith convergence in the older literature. See Kelley, Chapter 2, for additional discussion.

There is an alternate approach to convergence in topological spaces popularized by Bourbaki. For a discussion of this *theory of filters* see Choquet, §4, or Bourbaki, *Topologie générale*, Chapter 1. We find the filter theory of convergence very unintuitive and prefer the use of nets in all cases.

Section IV.3 It was Tychonoff who realized the utility of the product topology (and proved the Tychonoff theorem) in two fundamental papers: "Über die topologische Erweiterung von Räumen," *Math. Ann.* **102** (1929), 544–556, and "Über einen Funktionenraum," *Math. Ann.* **111** (1935), 762–766. The usual proof of Tychonoff's theorem (c.f. Kelley), depends on the f.i.p. criterion and is a little complicated. The machinery of filters, especially ultrafilters is ideal for a simpler looking proof of the theorem (cf. Choquet). This filter theoretic proof has a net theory translation which we should like to sketch. (1) A net $\{x_\alpha\}$ in a space X is called *universal* if for any $A \subset X$, $x_\alpha \in A$ eventually or $x_\alpha \in X \backslash A$ eventually. Note: A is arbitrary and the definition of universal net makes no mention of topology. (2) If x is a cluster point of a universal net, one has $x_\alpha \to x$, for it cannot happen that $x_\alpha \in A$ frequently without $x_\alpha \in A$ eventually. (3) Any net has a universal subnet. This is the technical heart of the proof and requires the axiom of choice. (4) X is compact if and only if every universal net converges. Given (3), this is just the Bolzano–Weierstrass theorem. (5) To prove Tychonoff's theorem, let $\{x_\alpha\}_{\alpha \in D}$ be a universal net in $\mathbf{X}_{i \in I} A_i$ with each A_i compact. Write $x_\alpha = \{x_\alpha^{(i)}\}_{i \in I}$ with $x_\alpha^{(i)} \in A_i$. Since $\{x_\alpha\}$ is universal, $\{x_\alpha^{(i)}\}$ is universal for each i. Since A_i is compact, $x_\alpha^{(i)} \to x^{(i)}$ for some $x^{(i)} \in A_i$. Let x be the element $\{x^{(i)}\}_{i \in I}$ in $\mathbf{X}_{i \in I} A_i$. Then $x_\alpha \to x$, so every universal net converges. We first learned this proof from O. E. Lanford, III, Les Houches lectures, 1970.

When does a topological space have a topology given by a metric? In general, there is not a simple answer, but for compact Hausdorff spaces, X is metrizable (has a topology given by a metric) if and only if it is second countable. In Section V.2, we see that a similar result holds for topological vector spaces. Both the compact and the vector space results are best understood in the context of uniform spaces; see Kelley, Chapter 6.

K. Weierstrass' original proof of the polynomial approximation theorem can be found on page 5 of Vol. 3 of his *Mathematische Werke*, Mayer and Müller, Berlin, 1903. Stone's generalization first appeared in M. H. Stone, "Applications of the Theory of Boolean Rings to General Topology," *Trans. Amer. Math. Soc.* **41** (1937), 325–481, and a simplified proof was given in his classic article "The Generalized Weierstrass Approximation Theorem," *Math. Mag.* **21** (1947/48), 167–184, 237–254.

Section IV.4 For a brief readable discussion of measure theory on compact spaces we especially recommend the first chapter of L. Nachbin, *The Haar Integral*, Van Nostrand–Reinhold, Princeton, New Jersey, 1965. For a more comprehensive discussion see N. Bourbaki, *Integration*, Chapters 1–4.

Much of our discussion on positive linear functionals goes through for vector spaces with an order allowing finite inf's and sup's, that is for vector lattices. For the deep relations between order notions and topology, see L. Nachbin, *Topology and Order*, Van Nostrand–Reinhold, Princeton, New Jersey, 1965.

For additional discussion of measure theory on locally compact spaces, see the quoted references of Nachbin and Bourbaki, or, for a discussion more similar to our approach, Choquet's book (see notes to Section IV.1).

Section IV.5 We will eventually prove a stronger result than our claim that the linear combinations of Dirac measures are vaguely dense in $\mathscr{M}(X)$. We will actually show that the

linear combinations in $\mathscr{M}_{+,1}(X)$ are vaguely dense in $\mathscr{M}_{+,1}(X)$. Thus any positive measure μ with $\mu(X) = 1$ can be vaguely approximated by measures $\sum_{n=1}^{N} t_n \delta_{x_n}$ with $0 \le t_n \le 1$, $\sum t_n = 1$. This will follow from the Krein–Milman theorem which we discuss in Section XIV.1. The Banach–Alaoglu theorem was proven in L. Alaoglu: "Weak Topologies of Normed Linear Spaces," *Ann. Math.* **41** (1940), 252–267.

Theorem IV.22 can be extended to an arbitrary separable Banach space. More generally, one has Pettis' theorem: A vector-valued function is strongly measurable if and only if it is weakly measurable and almost separably valued (in the sense that after changing f on a set of measure zero, Ran f is separable). This theorem was first proven in B. J. Pettis, "On Integration in Vector Spaces," *Trans. Amer. Math. Soc.* **44** (1938), 277–304.

One can define the integral of a strongly measurable function by methods analogous to the methods used for real-valued functions. This *Bochner integral* is discussed in K. Yosida, *Functional Analysis*, Springer, New York, 1965 and in many other texts. It was invented by S. Bochner in "Integration von Funktionen, deren Werte die Elemente eines Vektoraumes sind," *Fund. Math.* **20** (1933), 262–276. The Bochner integral obeys a norm dominated convergence theorem. Throughout this book, we use the weak integral defined by $\ell(\int f(x)\,d\mu) = \int \ell(f(x))\,d\mu$. The Bochner integral has nicer properties than this weak integral but we will not need these extra properties so we settle for the simpler weak integral.

PROBLEMS

1. Prove that the family of all topologies on a space is a complete lattice, that is, that any family of topologies has a least upper bound and a greatest lower bound.

2. (Kuratowski closure axioms) Show that the operation $A \mapsto \bar{A}$ in a topological space has the properties:

   (i) $\overline{(\bar{A})} = \bar{A}$
   (ii) $\overline{A \cup B} = \bar{A} \cup \bar{B}$
   (iii) $A \subset \bar{A}$
   (iv) $\overline{\varnothing} = \varnothing$

   Conversely, suppose that $^- : 2^X \to 2^X$ is given ($2^X \equiv$ all subsets of X) obeying (i)–(iv). Show the family of sets B with $\overline{X \backslash B} = X \backslash B$ forms a topology for which the closure operation is $^-$.
   Reference: Kelley, pp. 42–43.

3. (a) Let 2 be the topological space $\{0, 1\}$ with the discrete topology. Prove that a topological space X is connected if and only if any continuous function $f: X \to 2$ is constant.
   (b) Prove that any product of connected spaces is connected.
   (c) Let S be a topological space. Suppose that $A, B \subset S$ are connected in the relative topology and $A \cap B \neq \varnothing$; $A \cup B = S$. Show that S is connected.
   (d) Let S be a topological space. Suppose that $S = \bar{D}$ and D is connected. Prove that S is connected.
   (e) Prove that a continuous image of a connected space is connected.

(f) Prove the intermediate value theorem of freshman calculus, that is, if f is a continuous function on $[a, b]$, then for any $f(a) < x < f(b)$, there is a $c \in [a, b]$ with $f(c) = x$.
Hint: Use (a) to prove (b)–(e).

4. (a) A topological space X is called Lindelöf if every open cover has a countable subcover. Prove that any second countable space is Lindelöf.
(b) Prove that a second countable, regular (that is T_3) space is normal (that is T_4).
Reference: Kelley, pp. 49, 113.

5. (a) Prove that $\mathbb{R}$ and $\mathbb{R}^n$ are not homeomorphic for any $n > 1$.
(b) Prove that $\mathbb{R} \neq X \times X$ for any topological space X.
Hint: What happens to $\mathbb{R}$ if a single point is removed?

6. A topological space X is called arcwise connected if given $x, y \in X$, there is a continuous function (an arc!) f: $[0, 1] \to X$ with $f(0) = x$, $f(1) = y$.
(a) Show that if X is arcwise connected, it is connected.
(b) Let X_0 be the graph of the function $y = \sin 1/x$ on $\mathbb{R} - \{0\}$, given the relative topology as a subset of the plane. Let $X = X_0 \cup \{\langle x, y\rangle \mid x = 0\}$. Show that Y is connected but not arcwise connected.

7. Let $X = \mathbb{R}$ with the topology $\mathcal{T}$ generated by all sets of the form $\{[a, b) \mid a, b \in \mathbb{R}\}$ which is actually a base for $\mathcal{T}$. Prove that
(a) $\langle X, \mathcal{T}\rangle$ is separable.
(b) $\langle X, \mathcal{T}\rangle$ is first countable.
(c) $\langle X, \mathcal{T}\rangle$ is *not* second countable.

8. Prove that a subspace of a separable metric space is separable.

9. Let Y be $\mathbb{R}^2$ with the product topology given by taking the topology $\mathcal{T}$ of Problem 7 on each factor. Prove that:
(a) Y is separable.
(b) The line $x + y = 1$ is not separable in the relative topology.

10. Let X be any uncountable set and let $\mathcal{T}$ be the topology consisting of $\varnothing$ and complements of finite sets. Prove that
(a) X is separable.
(b) X is compact.
(c) X is T_1 but *not* T_2.
(d) X is neither first nor second countable.

†11. Prove Theorem IV.2.

12. Let X be the Banach space l_∞ and consider the sequence $\delta_1, \delta_2, \ldots$ in X^* given by

$$\delta_n(\{c_k\}_{k=1}^{\infty}) = c_n$$

Prove that $\{\delta_n\}, \ldots$ has no weak-* convergent subsequence but that it has a weak-* convergent subnet.

13. Give an example to show that a pointwise limit of a *net* of Borel functions on $\mathbb{R}$ may not be Borel.

14. Show that the space of the example in Section IV.2 is not compact but is Lindelöf (see Problem 4).

15. Let $\mathscr{A}$ be the family of continuous functions on $[0, 2\pi]$ with the property $\int_0^{2\pi} e^{ikx} f(x) = 0$ if k is a negative integer. Prove $\mathscr{A}$ is an algebra which is closed and separates points with $1 \in \mathscr{A}$ but for which $\mathscr{A} \neq C[0, 2\pi]$.

†*16.* Prove the conclusion of the Stone–Weierstrass theorem in the case where we do not suppose $1 \in \mathscr{B}$.

**17.* Let $\mathscr{B}$ be an ideal of $C_{\mathbb{R}}(X)$ which is closed. Let $Y = \{x \in X \mid f(x) = 0 \text{ for all } f \in \mathscr{B}\}$. Prove that Y is closed and that $\mathscr{B} = \{f \in C_{\mathbb{R}}(X) \mid f = 0 \text{ on } Y\}$.

18. Prove the Tietze theorem in the case when X is merely assumed normal. (See the hints given in Kelley, Chapter 7, Problem O.)

19. Let f be a continuous function on $[-\frac{1}{2}, \frac{1}{2}]$ with $f(\frac{1}{2}) = f(-\frac{1}{2}) = 0$. Let $s_k(x)$ be a sequence of functions with $\int_{-1}^{1} s_k(x)\,dx = 1$, each $s_k \geq 0$ so that for any $\delta > 0$,

$$\lim_{k \to \infty} \int_{1 \geq |x| \geq \delta} s_k(x) = 0$$

Prove that

$$\lim_{k \to \infty} \int_{-1/2}^{1/2} s_k(x - y) f(y)\,dy = f(x)$$

for any $x \in [-\frac{1}{2}, \frac{1}{2}]$ and that the convergence is uniform.

20. Let $s_k(x) = (I_k)^{-1}(1 - x^2)^k$ where $I_k = \int_{-1}^{1} (1 - x^2)^k\,dx$. Using Problem 19, prove that any continuous function on $[-\frac{1}{2}, \frac{1}{2}]$ is a limit of polynomials uniformly on $[-\frac{1}{2}, \frac{1}{2}]$.

21. Use the Stone–Weierstrass theorem to prove that:
(a) $\{e^{ikx}\}_{k=-\infty}^{\infty}$ are a complete *orthogonal* set for $L^2[0, 2\pi]$.
(b) The Legendre polynomials are a complete *orthogonal* set for $L^2[-1, 1]$.
*(c) The spherical harmonics are a complete orthonormal set for L^2 of the sphere. (Hint: Use your knowledge of Clebsch–Gordon coefficients!)

22. Prove *Dini's theorem*: Let X be a compact Hausdorff space. Suppose f_n is a monotone decreasing family of functions; let $f_n(x) \to f(x)$ pointwise. Then f_n converges uniformly if and only if f is continuous.

23. Let X be a locally compact Hausdorff space. Consider $\hat{X} = X \cup \{\infty\}$ where ∞ is a "point" not in X. Call $O \subset \hat{X}$ open if either $\infty \notin O$ and O is open in X or $\infty \in O$ and $\hat{X} \backslash O$ is compact. Prove that $\hat{X}$ is a compact Hausdorff space; it is called the **one-point compactification** of X.

24. Prove the Stone–Weierstrass theorem for a locally compact space X: If $\mathscr{A}$ is a closed subalgebra of $C_\infty(X)$, the continuous real-valued functions vanishing at ∞, and if $\mathscr{A}$ separates points and for each $x \in X$, there is $f \in \mathscr{A}$ with $f(x) \neq 0$, then $\mathscr{A} = C_\infty(X)$.

25. Let X be a locally compact Hausdorff space. Prove that for $C, D \subset X$, D closed, C compact, there is a continuous function f, $0 \le f \le 1$, on X with $f[C] = 0$, $f[D] = 1$.
Remark. Use the space $\hat{X}$ of Problem 23 to solve 24 and 25.

26. (a) Prove that any locally compact Hausdorff space is T_3.
(b) Prove that any second countable, locally compact Hausdorff space is normal.
(c) Prove that any σ-compact, locally compact Hausdorff space is normal.
Remark. There exist locally compact spaces which are Hausdorff but not normal, see Kelley, Chapter 4, Problem E.

27. A group G with a topology is called a topological group if the map $\langle x, y\rangle \mapsto xy^{-1}$ of $G \times G \to G$ is jointly continuous. A function f on a topological group G is called uniformly continuous if, for any ε, we can find a neighborhood N_ε of $e \in G$ (the identity) with $|f(x) - f(y)| < \varepsilon$ if $xy^{-1} \in N_\varepsilon$. Prove that any continuous function on a compact topological group is uniformly continuous.

*28. (a) Let $\mathscr{A}$ be an algebra of real-valued bounded continuous functions on $\mathbb{R}$ which separates points and is closed in $\|\cdot\|_\infty$. Form $X_{\mathscr{A}} \equiv \times_{f\in\mathscr{A}} \{x \in \mathbb{R} \mid |x| \le \|f\|_\infty\}$ with the product topology. Map $\mathbb{R} \to X_{\mathscr{A}}$ by letting x go into the point whose coordinates are $\{f(x)\}_{f\in\mathscr{A}}$. Prove that the image of $\mathbb{R}$ in $X_{\mathscr{A}}$ is homeomorphic to $\mathbb{R}$ if and only if $\mathscr{A}$ contains the functions of compact support.
(b) A topological space X with a map $f: \mathbb{R} \to X$ is called a **compactification** of $\mathbb{R}$ if f is a homeomorphism of $\mathbb{R}$ and its image, if the image is dense in X and if X is a compact Hausdorff space. Two compactifications $f: \mathbb{R} \to X$ and $g: \mathbb{R} \to Y$ are considered identical if there is a homeomorphism $h: X \to Y$ with $h \circ f = g$. Prove that there is a one-one correspondence between compactifications of $\mathbb{R}$ and algebras $\mathscr{A} \subset C_{\mathbb{R}}$ obeying the conditions of (a).
(c) If we take $\mathscr{A} = C(\mathbb{R})$, the compactification we obtain via the construction in (a) is called the **Stone-Čech compactification**, $\check{\mathbb{R}}$. Prove that $\check{\mathbb{R}}$ is a universal compactification of $\mathbb{R}$ in the following sense: Given any compactification $f: \mathbb{R} \to X$ and given the Stone-Čech compactification $g: \mathbb{R} \to \check{\mathbb{R}}$ we can find $h: \check{\mathbb{R}} \to X$ continuous and surjective with $h \circ g = f$.

29. Let $\langle X, d\rangle$ be a metric space with no isolated points. Suppose that every continuous function on X is uniformly continuous. Show that X is compact.

30. (a) Prove that every metric space is normal.
(b) Prove that every closed set in a metric space is a G_δ.

†31. Prove the uniqueness statement of Theorem IV.16.

32. Let $\{a_n\}$ be a sequence of numbers with the following property: If $\sum_{n=0}^{N} \alpha_n x^n \ge 0$ for all $x \in [0, 1]$ then $\sum_{n=0}^{N} \alpha_n a_n \ge 0$. Prove that there is a unique, (positive) measure μ on $[0, 1]$ with $a_n = \int_0^1 x^n \, d\mu$.

33. Let X be a vector space with Y a family of functionals separating points. Prove that if the $\sigma(X, Y)$ topology comes from a metric, then Y has a countable *algebraic* dimension. An **algebraic basis** for Y is a subset whose *finite* linear combinations span Y. The **algebraic dimension** is the number of elements in a minimal algebraic basis.

34. Let X be a real Banach space and let C be the unit ball of X^* with the weak-* topology. Prove that a continuous function on C can be uniformly approximated by polynomials in the elements of X acting as linear functionals on X^*.

35. Let X be a Banach space, X^* its dual. Let L_n, $n \geq 1$ be elements of X^* with $L_n \to L \in X^*$ in the weak-* sense. Let $x_n \to x$ in norm. Is it necessarily true that $L_n(x_n) \to L(x)$?

36. Prove that X is dense in X^{**} in the $\sigma(X^{**}, X^*)$ topology.

37. Let T: $C(X) \to C(Y)$ be linear. We say T is positivity preserving (or positive) if $Tf \geq 0$ whenever $f \geq 0$. If T is positive, we write $T \geq 0$. If $S - T \geq 0$ we write $T \leq S$.
(a) Prove that any $T \geq 0$ is automatically continuous and that $\|T\| = \|T1\|_\infty$.
(b) Let S_n be an increasing family of maps. Prove that S_n converges in operator norm if and only if $S_n 1$ converges in function norm.

†*38.* Prove the first proposition in Section IV.2.

†*39.* Find a Banach space and a weakly convergent net which is not norm bounded.

†*40.* Let X be an infinite-dimensional Banach space with the weak topology. Prove that the closure of the unit sphere is the unit ball.

†*41.* Let X be a compact Hausdorff space. Prove that the set of convergent infinite linear combinations of point measures is norm closed in $\mathcal{M}(X)$.

†*42.* Prove Theorem IV.19 directly.

**43.* (a) Let X be a compact set with a countable basis. Let μ be a Baire measure on X. Prove that $L^p(X, d\mu)$ is separable for all $p < \infty$. (Hint: Let A_n be a countable basis of sets. For all n, m with $\bar{A}_n \cap \bar{A}_m = \varnothing$, find $f_{n,m} \in C(X)$ with $f = 0$ on A_n, $f = 1$ on A_m. Use the $f_{n,m}$ to construct a countable dense set in $C(X)$. Then use the fact that $C(X)$ is dense in $L^p(X, d\mu)$).
(b) Extend the result of (a) to the case where X is only locally compact (Hint: Prove that X is σ-compact).

**44.* Do any fifty problems in Kelley's book.

V: Locally Convex Spaces

Mathematicians are like Frenchmen: whatever you say to them they translate into their own language and forthwith it is something entirely different. *J. W. Goethe*

V.1 General properties

We have already discussed several nonnormed topologies on vector spaces in the investigation of weak topologies in Section IV.5. We have also alluded to the fact that if X is a locally compact topological space, the Baire measures on X are the dual space of the continuous functions of compact support, $\kappa(X)$, when it is given a suitable nonnormed topology. Our goal in this chapter is to discuss a general class of topologized vector spaces which includes these examples and also the spaces of distributions which arise in a wide variety of functional situations and physical problems.

The idea behind the topologies we discuss is quite simple. Suppose that, instead of one norm, we have a family of norms $\{\rho_\alpha\}_{\alpha \in A}$ where A is some index set. We should like a topology in which a net $\{x_\beta\}$ converges to x if and only if $\rho_\alpha(x_\beta - x) \to 0$ for each fixed $\alpha \in A$. However, it is useful to weaken one condition on the norm. Recall that $\|x\| = 0$ implies $x = 0$ and that this condition is needed for limits to be unique, that is, for the induced topology to be Hausdorff. Suppose that $\{\rho_\alpha\}_{\alpha \in A}$ is a family of objects obeying all the norm conditions except $x = 0$ when $\rho_\alpha(x) = 0$ for some α. But suppose instead that $x = 0$ whenever $\rho_\alpha(x) = 0$ for all α; then it is easy to see

limits are unique in a topology where convergence means $\rho_\alpha(x_\beta - x) \to 0$ for each fixed α. We thus define:

Definition A **seminorm** on a vector space V is a map $\rho: V \to [0, \infty)$ obeying:

(i) $\rho(x + y) \leq \rho(x) + \rho(y)$
(ii) $\rho(\alpha x) = |\alpha|\rho(x)$ for $\alpha \in \mathbb{C}$ (or $\mathbb{R}$).

A family of seminorms $\{\rho_\alpha\}_{\alpha \in A}$ is said to **separate points** if

(iii) $\rho_\alpha(x) = 0$ for all $\alpha \in A$ implies $x = 0$.

Definition A **locally convex space** is a vector space X (over $\mathbb{R}$ or $\mathbb{C}$) with a family $\{\rho_\alpha\}_{\alpha \in A}$ of seminorms separating points. The **natural topology** on a locally convex space is the weakest topology in which all the ρ_α are continuous and in which the operation of addition is continuous.

We temporarily defer giving examples or the explanation of the term "locally convex." We also note that many authors do not require the seminorms to separate points but add it as an extra condition. The significance of the separation condition is that it implies (Problem 6a):

Proposition The natural topology of a locally convex space (with our definition!) is Hausdorff.

A neighborhood base at 0 for the natural topology is given by the sets $\{N_{\alpha_1, \ldots, \alpha_n; \varepsilon} | \alpha_1, \ldots, \alpha_n \in A; \varepsilon > 0\}$ where

$$N_{\alpha_1, \ldots, \alpha_n; \varepsilon} = \{x | \rho_{\alpha_i}(x) < \varepsilon, i = 1, \ldots, n\}$$

Thus, a net $x_\beta \to x$ if and only if $\rho_\alpha(x_\beta - x) \to 0$ for all $\alpha \in A$. The notion of completeness extends naturally:

Definition A net $\{x_\beta\}$ in a locally convex space X is called **Cauchy** if and only if, for all $\varepsilon > 0$, and for each seminorm ρ_α there is a β_0 so that $\rho_\alpha(x_\beta - x_\gamma) < \varepsilon$ if $\beta, \gamma > \beta_0$. X is called **complete** if every Cauchy net converges.

The important structure on a locally convex space is the natural topology rather than the particular seminorms used to generate the topology. We call

two families of seminorms $\{\rho_\alpha\}_{\alpha \in A}$ and $\{d_\beta\}_{\beta \in B}$ on a vector space X **equivalent** if they generate the same natural topology. It is often useful to know (Problem 6b):

Proposition Let $\{\rho_\alpha\}_{\alpha \in A}$ and $\{d_\beta\}_{\beta \in B}$ be two families of seminorms. The following statements are equivalent:

(a) The families are equivalent families of seminorms.

(b) Each ρ_α is continuous in the d-natural topology and each d_β is continuous in the ρ-natural topology.

(c) For each $\alpha \in A$, there are $\beta_1, \ldots, \beta_n \in B$ and $C > 0$ so that for all $x \in X$

$$\rho_\alpha(x) \leq C(d_{\beta_1}(x) + \cdots + d_{\beta_n}(x))$$

and for each $\beta \in B$, there are $\alpha_1, \ldots, \alpha_m \in A$ and $D > 0$ so that for all $x \in X$

$$d_\beta(x) \leq D(\rho_{\alpha_1}(x) + \cdots + \rho_{\alpha_m}(x))$$

The appearance of expressions like $C(d_{\beta_1}(x) + \cdots + d_{\beta_n}(x))$ is quite common in the theory of locally convex spaces. It is thus useful to consider families of seminorms with a special property:

Definition A family $\{\rho_\alpha\}_{\alpha \in A}$ of seminorms on a vector space V is called **directed** if and only if for all $\alpha, \beta \in A$ there is a $\gamma \in A$ and a C so that

$$\rho_\alpha(x) + \rho_\beta(x) \leq C\rho_\gamma(x)$$

for all $x \in V$. Equivalently, by induction, for all $\alpha_1, \ldots, \alpha_n \in A$ there is a γ and D so that

$$\rho_{\alpha_1}(x) + \cdots + \rho_{\alpha_n}(x) \leq D\rho_\gamma(x)$$

for all $x \in V$.

For example, if $\{\rho_\alpha\}_{\alpha \in A}$ is a directed family, then $\{\{x \mid \rho_\alpha(x) < \varepsilon\} \mid \alpha \in A, \varepsilon > 0\}$ is a neighborhood base at 0. One can always find directed sets of seminorms:

Proposition Every locally convex space has a directed family of seminorms equivalent to the family defining the space.

Proof If $\{\rho_\alpha\}_{\alpha \in A}$ defines the space, let B be the set of finite subsets of A. If $F \in B$, let $d_F = \sum_{\alpha \in F} \rho_\alpha$. Then $\{d_F\}_{F \in B}$ is directed and equivalent to the initial set. ∎

We consider briefly two examples. In Sections V.3 and V.4 we will discuss several other examples; in particular, the technical appendix of Section V.3 is useful to the reader desiring experience with equivalent semi-norms and directed sets of seminorms.

Example 1 Let X be a vector space and suppose that Y is a set of linear functionals on X separating points. In Section IV.5, we introduced the $\sigma(X,Y)$-topology. It is precisely the locally convex topology generated by the seminorms $\{\rho_\ell | \ell \in Y\}$ where $\rho_\ell(x) = |\ell(x)|$. While this topology is given by seminorms, it is never given by norms if Y has infinite algebraic dimension (Problem 2).

Example 2 Let D be a region of the complex plane, that is, D is connected and open. Let $\mathcal{O}_D$ be the vector space of all (single-valued) analytic functions in D. For any compact $C \subset D$, let $\rho_C(f) = \sup_{z \in C} |f(z)|$. $\mathcal{O}_D$, topologized by the seminorms ρ_C, is a locally convex space which is complete. For suppose f_α is a ρ_C-Cauchy net for all C. Then, $f_\alpha(z) \to f(z)$ uniformly on compacts sets. By a classical theorem of Weierstrass, f is analytic (essentially because f is analytic if and only if it obeys the Cauchy integral formula which is preserved by uniform limits). Let

$$\rho_C^{(2)}(f) = \iint_{x+iy \in C} |f(x+iy)|^2 \, dx \, dy$$

The families $\{\rho_C^{(2)}\}$ and $\{\rho_C\}$ are equivalent families (Problem 7).

We are now prepared to discuss the reason for the name locally convex and the associated geometrical ideas and construction. The neighborhoods $N_{\alpha_1,\alpha_2,\ldots,\alpha_n;\varepsilon}$ have special geometric properties:

Definition A set $C \subset V$, a vector space, is called **convex** if x and $y \in V$, $0 \leq t \leq 1$, implies $tx + (1-t)y \in C$. C is called **balanced** (or **circled**) if $x \in C$ and $|\lambda| = 1$ implies $\lambda x \in C$. Finally, C is called **absorbing** (or **absorbent**) if $\bigcup_{t>0} tC = V$, that is, if for every $x \in V$, $sx \in C$ for some $s > 0$.

If C is convex and V is a vector space over the reals, balanced means only that $-x \in C$ whenever $x \in C$; if V is a vector space over the complex numbers, balanced means $e^{i\theta}x \in C$ whenever $\theta \in [0, 2\pi)$ and $x \in C$ (so circled is a more suitable name).

It is an elementary application of the definitions to see that the $N_{\alpha_1,\ldots,\alpha_n;\varepsilon}$ are convex; in fact:

Proposition If $\rho_{\alpha_1}, \ldots, \rho_{\alpha_n}$ are seminorms on a vector space V then $\{x \mid |\rho_{\alpha_1}(x)| < \varepsilon, \ldots, |\rho_{\alpha_n}(x)| < \varepsilon\}$ is a balanced, convex, absorbing set.

This proposition is a one-half of the basic theorem:

Theorem V.1 Let V be a vector space with a Hausdorff topology in which addition and scalar multiplication are separately continuous. Then V is a locally convex space (that is, has a topology given by a family of seminorms) if and only if 0 has a neighborhood base of balanced, convex, absorbing sets.

The proof of the other half of the theorem, that is, that V has a topology generated by seminorms if 0 has a neighborhood base of balanced, convex, absorbing sets relies on the following technical device:

Definition Let C be an absorbing subset of a vector space V with the additional property that if $x \in C$ and $0 \leq t \leq 1$, then $tx \in C$. The **Minkowski functional** or **gauge** of C is the map $\rho: V \to [0, \infty)$ given by

$$\begin{aligned}\rho(x) &= \inf\{\lambda \mid x \in \lambda C\} \\ &= [\sup\{\mu \mid \mu x \in C\}]^{-1}\end{aligned}$$

Lemma

(a) If $t \geq 0$, then $\rho(tx) = t\rho(x)$ for the gauge of any set C.
(b) ρ obeys $\rho(x + y) \leq \rho(x) + \rho(y)$ if C is convex.
(c) ρ obeys $\rho(\lambda x) = |\lambda|\rho(x)$ if C is circled.
(d) $\{x \mid \rho(x) < 1\} \subset C \subset \{x \mid \rho(x) \leq 1\}$.

The proof of this beautiful lemma is left to the problems.

Proof of Theorem V.1 Let $\mathscr{U}$ be a neighborhood base at 0 containing only convex, balanced, absorbing sets; for each $U \in \mathscr{U}$, let ρ_U be the gauge of U. By (b) and (c) of the lemma, ρ is a seminorm and by (d) the neighborhoods of 0 in the original topology are the same as those in the locally convex topology given by the seminorms $\{\rho_U \mid U \in \mathscr{U}\}$. Since addition is separately continuous in both topologies, the neighborhoods about any point are identical in the two topologies. ∎

In normed linear spaces, a linear map from X to Y is continuous if and only if it is bounded. A similar result holds in locally convex spaces (Problem 9):

Theorem V.2 Let X and Y be locally convex spaces with families of semi-norms $\{\rho_\alpha\}_{\alpha \in A}$ and $\{d_\beta\}_{\beta \in B}$. Then a linear map $T: X \to Y$, is continuous if and only if for all $\beta \in B$, there are $\alpha_1, \ldots, \alpha_n \in A$ and $C > 0$ with

$$d_\beta(Tx) \leq C(\rho_{\alpha_1}(x) + \cdots + \rho_{\alpha_n}(x))$$

If the $\{\rho_\alpha\}_{\alpha \in A}$ are directed, then T is continuous if and only if for all $\beta \in B$

$$d_\beta(Tx) \leq D\rho_\alpha(x)$$

for some $\alpha \in A$, and $D > 0$.

Finally, we conclude this introduction by discussing two applications of the Hahn–Banach theorem (Theorem III.5) to locally convex spaces. First:

Theorem V.3 Let X be a locally convex space and let $Y \subset X$ be a subspace. Let $\ell: Y \to \mathbb{R}$ (or $\mathbb{C}$ if X is a complex space) be linear and continuous. Then, there is a continuous linear map $L: X \to \mathbb{R}$ (or $\mathbb{C}$) with $L \restriction Y = \ell$.

Proof The relative topology on Y is given by the restrictions of the continuous seminorms to Y. Thus, $|\ell(x)| \leq C\rho(x)$ for some continuous seminorm. Applying Theorem III.5 or III.6, we obtain our result. ∎

Thus, locally convex spaces possess many continuous linear functionals; in fact, enough to separate points. We denote by X^* the family of continuous linear functionals on X and call it the **topological dual**.

The second application of the theorem is more geometric in nature and is related to the idea of slipping a closed hyperplane between disjoint convex sets; see Figure V.1. A **hyperplane** is the set of points where $\ell(x) = a$ for some *real-valued* linear functional (even in the complex case).

Definition We say that two sets A and B in a locally convex space are **separated by a hyperplane** if there is a continuous real-valued functional ℓ and an $a \in \mathbb{R}$ with $\ell(x) \leq a$ for $x \in A$ and $\ell(x) \geq a$ for $x \in B$. If $\ell(x) < a$ for $x \in A$ and $\ell(x) > a$ for $x \in B$, we say that A and B are **strictly separated**.

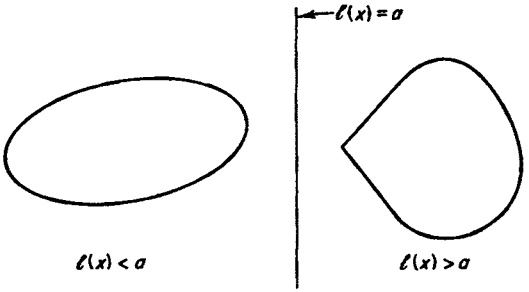

FIGURE V.1

Theorem V.4 (Separating hyperplane theorem) Let A and B be disjoint convex sets in a locally convex space X. Then:

(a) If A is open, they can be separated by a hyperplane.

(b) If A and B are both open, they can be strictly separated by a hyperplane.

(c) If A is compact and B is closed, they can be strictly separated by a hyperplane.

Proof (a) Pick $-x \in A - B = \{y - z \mid y \in A, z \in B\}$. Let $C = A - B + \{x\}$. Then C is open and thus absorbing, convex, $0 \in C$ and $x \notin C$ since A and B are disjoint. Let ρ_C be the Minkowski functional for C. Then $\rho_C(z + y) \leq \rho_C(z) + \rho_C(y)$ and $\rho_C(az) = a\rho_C(z)$ if $a > 0$. Define ℓ on $\{\lambda x \mid \lambda \in \mathbb{R}\}$ by $\ell(\lambda x) = \lambda$. Since $x \notin C$, $\rho_C(x) \geq 1$ so that $\ell(x) \leq \rho_C(x)$. Thus, by Theorem III.5, ℓ has an extension to all of X with $\ell(y) \leq \rho_C(y)$. Since $C \cap (-C) \subset \ell^{-1}[-1, 1]$, ℓ is continuous. By the inequality, $\ell(y) \leq 1$ if $y \in C$. Thus for any $a \in A$ and $b \in B$, $\ell(a) \leq \ell(b) + (1 - \ell(x))$. Since $\ell(x) = 1$,

$$\sup_{a \in A} \ell(a) \leq \inf_{b \in B} \ell(b)$$

so ℓ separates A and B.

(b) It is easy to see that if ℓ is a nonzero linear functional and A is open, then $\ell[A]$ is open. Since $\ell[A]$ and $\ell[B]$ are open and intersect in at most one point, they are automatically disjoint.

(c) Since A and B are disjoint, $0 \notin B - A \equiv S$. Since A is compact, it is easy to see that S is closed. Thus there is an open convex set U disjoint from S with $0 \in U$. Let $A' = A + \frac{1}{2}U$ and $B' = B - \frac{1}{2}U$. Then A' and B' are disjoint, open, convex sets that may be strictly separated by a hyperplane by (b). Since $A \subset A'$ and $B \subset B'$, this hyperplane also separates A and B. ∎

In Chapter XIV we will discuss an "algebraic Hahn–Banach theorem," i.e. a form of the separation theorem which makes no mention of open sets or continuous functions.

V.2 Fréchet spaces

In Section III.5, we saw that complete metric spaces have special properties which imply strong results for Banach spaces. It is thus of interest to single out those locally convex spaces that are also complete metric spaces. First, we must ask which locally convex spaces are metrizable, that is, have a topology generated by a metric. These are not only the spaces whose topology is given by a norm, for if ρ is a metric, $\rho(x, 0)$ need not be a norm since $\rho(\lambda x, 0)$ need not equal $\lambda\rho(x, 0)$.

Theorem V.5 Let X be a locally convex space. The following are equivalent:

(a) X is metrizable.

(b) 0 has a countable neighborhood base.

(c) The topology on X is generated by some countable family of seminorms.

Proof We show (a) $\Rightarrow$ (b) $\Rightarrow$ (c) $\Rightarrow$ (a).

(a) $\Rightarrow$ (b) is a property of any metric space.

(b) $\Rightarrow$ (c) follows from the fact that if $\mathscr{U}$ is any neighborhood base of convex, balanced sets, the gauges of $U \in \mathscr{U}$ generate the topology and the fact that if 0 has a countable neighborhood base, we can find a countable neighborhood base of convex, balanced sets.

(c) $\Rightarrow$ (a). Let $\{\rho_n\}_{n=1,2,\ldots,}$ be a family of seminorms generating the topology. Define ρ on $X \times X$ by

$$\rho(x, y) = \sum_{n=1}^{\infty} 2^{-n}\left[\frac{\rho_n(x - y)}{1 + \rho_n(x - y)}\right] \tag{V.1}$$

Since $a/(1 + a) < 1$ for any $a > 0$, $\rho(x, y) < \infty$. It is easy to see that ρ is a metric and that it generates the same topology as the $\{\rho_n\}_{n=1}^{\infty}$ (Problem 10a). ∎

In addition, the two notions of complete are the same (Problem 10b):

Proposition A net $\{x_\alpha\}$ is Cauchy in the metric ρ of (V.1) if and only if it is Cauchy in each ρ_n. Thus a metrizable locally convex space X is complete as a metric space if and only if it is complete as a locally convex space.

Definition A complete metrizable locally convex space is called a **Fréchet space**.

As complete metric spaces, Fréchet spaces obey the Baire category theorem, and thus one can prove theorems analogous to those found in Section III.5:

Theorem V.6 If X and Y are Fréchet spaces and $f: X \to Y$ is a continuous linear surjection, then f is open.

Theorem V.7 Let X and Y be Fréchet spaces; let $\mathscr{F}$ be a family of continuous linear maps from X to Y so that for continuous seminorm ρ on Y and every $x \in X$, $\{\rho(F(x)) \mid F \in \mathscr{F}\}$ is bounded. Then, for each ρ there is a continuous seminorm d on X and a $C > 0$ so that

$$\rho(Fx) \leq Cd(x)$$

for all $x \in X$ and $F \in \mathscr{F}$.

For an application of Theorem V.6, see Problem 12. As an application of Theorem V.7, we first notice that the corollary of Theorem III.9 goes through without change:

Corollary If X is a Fréchet space, a separately continuous bilinear functional, B, is jointly continuous, that is, $|B(f, g)| \leq C\rho_1(f)\rho_2(g)$ for some continuous seminorms ρ_1, ρ_2.

We can also prove the following corollary of Theorem V.7 whose proof can be viewed as Theorem I.27 in disguise:

Theorem V.8 Let X be a Fréchet space and let $f_n \in X^*$ be a *sequence* converging to $f \in X^*$ in the $\sigma(X^*, X)$-topology. Then $f_n \to f$ uniformly on compact subsets of X.

Proof Since $f_n(x)$ is convergent, it is bounded, so we can find a continuous seminorm ρ on X so that $|f_n(x)| \leq C\rho(x)$. Given a compact subset D of X, and an ε, pick a finite cover of D by sets $U_1, \ldots, U_m$ so that $x, y \in U_k$ implies

$\rho(x-y) \le \varepsilon/3C$. Now pick $x_k \in U_k$ and N so $n > N$ implies $|f_n(x_i) - f(x_i)| < \varepsilon/3$ for $i = 1, \ldots, m$. Then an $\varepsilon/3$ argument proves

$$\sup_{x \in D} |f_n(x) - f(x)| < \varepsilon \qquad \text{if} \quad n > N \ \blacksquare$$

V.3 Functions of rapid decrease and the tempered distributions

We want to discuss a very convenient space of functions, the functions of rapid decrease $\mathscr{S}$ and its dual, the tempered distributions. To make the definitions flow more smoothly, we first introduce some notation. We will write functions on $\mathbb{R}^n$ merely as $f(x)$, $x = \langle x_1, \ldots, x_n \rangle$. I_+^n will always denote the set of all n-tuples of nonnegative integers $\alpha = \langle \alpha_1, \ldots, \alpha_n \rangle$ and $|\alpha| = \sum_{i=1}^n \alpha_i$; $I_+^1 = I_+$. Further,

$$D^\alpha \qquad \text{will denote} \qquad \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}$$

and x^α denotes $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$.

Definition The **functions of rapid decrease** $\mathscr{S}(\mathbb{R}^n)$ is the set of infinitely differentiable complex-valued functions $\varphi(x)$ on $\mathbb{R}^n$ for which

$$\|\varphi\|_{\alpha,\beta} \equiv \sup_{x \in \mathbb{R}^n} |x^\alpha D^\beta \varphi(x)| < \infty$$

for all $\alpha, \beta \in I_+^n$.

Thus, the functions in $\mathscr{S}$ are those functions which together with their derivatives fall off more quickly than the inverse of any polynomial.

Theorem V.9 The vector space $\mathscr{S}(\mathbb{R}^n)$ with the natural topology given by the seminorms $\|\cdot\|_{\alpha,\beta}$ is a Fréchet space.

Proof The reader can easily check that $\|\cdot\|_{\alpha,\beta}$ is a seminorm. Since there are countably many of them, $\mathscr{S}(\mathbb{R}^n)$ is metrizable (Theorem V.5). Thus we need only show that $\mathscr{S}(\mathbb{R}^n)$ is complete. Suppose that f_m is Cauchy in each $\|\cdot\|_{\alpha,\beta}$. Then $x^\alpha D^\beta f_m \to g_{\alpha,\beta}$ uniformly as $m \to \infty$ since $C(\mathbb{R}^n)$ is complete. If we can show $g = g_{0,0}$ is C^∞ and $g_{\alpha,\beta} = x^\alpha D^\beta g$, then g will be in $\mathscr{S}$ and $\lim_{m\to\infty} f_m$

will be g in the topology of $\mathscr{S}$. Let us prove that g is C^1 and $dg/dx = g_{0,1}$ in the case of $\mathscr{S}(\mathbb{R}^1)$. The general case is proven by similar means. We know that

$$f_n(x) = f_n(0) + \int_0^x f_n'(t)\,dt$$

Since $f_n' \to g_{0,1}$ uniformly,

$$g(x) = g(0) + \int_0^x g_{0,1}(t)\,dt$$

Thus g is C^1 and $g' = g_{0,1}$. ∎

For technical reasons, we often want a directed family of seminorms, so we define for $k, m \in I_+$ and $f \in \mathscr{S}(\mathbb{R}^n)$,

$$\|f\|_{k,m} = \sum_{\substack{|\alpha| \le k \\ |\beta| \le m}} \|f\|_{\alpha,\beta}$$

Definition The (topological) dual space of $\mathscr{S}(\mathbb{R}^n)$, denoted by $\mathscr{S}'(\mathbb{R}^n)$, is called **the space of tempered distributions.**

For a linear functional T on $\mathscr{S}(\mathbb{R}^n)$ to be in $\mathscr{S}'(\mathbb{R}^n)$, it must be continuous. By Theorem V.2, this is equivalent to the existence of a seminorm $\|\cdot\|_{k,m}$ with $|T(\varphi)| \le C\|\varphi\|_{k,m}$ for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$. We discuss several examples in the case $n = 1$; the reader can easily extend them to the case of general n.

Example 1 ($\mathscr{S}$) Let $g \in \mathscr{S}(\mathbb{R}^1)$ and define a functional $g(\cdot)$ on $\mathscr{S}$ by

$$g(\varphi) = \int_{-\infty}^{\infty} g(x)\varphi(x)\,dx \tag{V.2}$$

$g(\cdot)$ is clearly linear and

$$|g(\varphi)| \le \|g\|_{L^1(\mathbb{R})}\|\varphi\|_\infty$$

and $\|\varphi\|_\infty$ is a continuous seminorm. Moreover, if $g_1 \neq g_2$ as functions in $\mathscr{S}$, $g_1(\cdot) \neq g_2(\cdot)$ as elements in $\mathscr{S}'$. For $\mathscr{S}$ is dense in L^2 so that $g_1 \neq g_2$ in $\mathscr{S}$ implies $g_1 \neq g_2$ in L^2 implies $g_1 \neq g_2$ in $(L^2)^*$ implies $g_1 \neq g_2$ in $\mathscr{S}'$.

We thus see that $\mathscr{S}$ is embedded naturally in $\mathscr{S}'$. This imbedding is continuous when $\mathscr{S}'$ is given the $\sigma(\mathscr{S}', \mathscr{S})$ topology since we will see that $\|\cdot\|_{L^1(\mathbb{R})}$ is a continuous seminorm on $\mathscr{S}$. Moreover, $\mathscr{S}$ is dense in $\mathscr{S}'$ in the

$\sigma(\mathscr{S}', \mathscr{S})$ topology (see Problems 16 and 19 or Corollary 1 to Theorem V.14 in the appendix to this section). This suggests extending continuous maps $T: \mathscr{S} \to \mathscr{S}$ to $\mathscr{S}'$ as follows: Since the natural map ι of $\mathscr{S} \to \mathscr{S}'$ is continuous $\iota \circ T: \mathscr{S} \to \mathscr{S}'$ is continuous from $\mathscr{S}$ to $\mathscr{S}'$. Since $\mathscr{S}$ is dense in $\mathscr{S}'$, there is at most one continuous extension of $\iota \circ T: \mathscr{S}' \to \mathscr{S}'$. To find this continuous extension we need some way of constructing continuous maps of $\mathscr{S}' \to \mathscr{S}'$. There is one simple method. Suppose $S: \mathscr{S} \to \mathscr{S}$ is continuous. Define the **adjoint** $S': \mathscr{S}' \to \mathscr{S}'$, $\ell \mapsto S'(\ell)$, by requiring that $[S'(\ell)](g) = \ell(Sg)$ for all g in $\mathscr{S}$. It is evident that if $\ell_\alpha \to \ell$ in the $\sigma(\mathscr{S}', \mathscr{S})$ topology, then $S'(\ell_\alpha) \to S'(\ell)$ in the $\sigma(\mathscr{S}', \mathscr{S})$ topology. Thus, to extend T, we seek a map $S: \mathscr{S} \to \mathscr{S}$ so that $S' \restriction \mathscr{S} = T$ and then extend T by using S'. When no confusion arises, we will denote this extension also by T. Adjoints are further discussed in Section VI.2.

This idea will become clearer as we discuss examples below. We will discuss another topology on $\mathscr{S}'$ in Section V.7 (the $\beta(\mathscr{S}', \mathscr{S}) \equiv \tau(\mathscr{S}', \mathscr{S})$ topology) and we will see that the adjoints S' are continuous when this topology is put on both the domain and range (see Problem 17).

Example 2 (L^p) $\mathscr{S}$ is a subset of each $L^p(\mathbb{R})$ and the identity mapping of $\mathscr{S}$ into L^p is continuous. For $p = 1$, we note that

$$\|f\|_1 = \int_{-\infty}^{\infty} (1 + x^2)^{-1}[(1 + x^2)|f|]\,dx \leq \pi(\|f\|_\infty + \|x^2 f\|_\infty)$$

and for general p, we notice that

$$\|f\|_p \leq \||f|^{1/p}|f|^{1-1/p}\|_p \leq \|f\|_1^{1/p}\|f\|_\infty^{1-1/p}$$

If $g \in L^q$, $q^{-1} + p^{-1} = 1$ and $\varphi \in \mathscr{S}$ we have

$$\left|\int g(x)\varphi(x)\,dx\right| \leq \|g\|_q\|\varphi\|_p$$

Thus $\varphi \to \int g(x)\varphi(x)\,dx$ is a continuous map of $\mathscr{S}$ into $\mathbb{C}$. This defines a continuous imbedding of L^q into $\mathscr{S}'$.

Thus $\mathscr{S}'$ contains the images of many spaces of functions under natural injections. We usually ignore the injections and refer to the function $g(x) \in \mathscr{S}'$.

Example 3 (the delta function) Let $b \in \mathbb{R}$. Define δ_b to be the linear functional $\delta_b(\varphi) = \varphi(b)$. Since $|\delta_b(\varphi)| \leq \|\varphi\|_{0,0}$, $\delta_b(\cdot) \in \mathscr{S}'(\mathbb{R})$. There is no

function $g(x)$ with $\delta_b(\varphi) = \int g(x)\varphi(x)\,dx$ for all $\varphi \in \mathscr{S}$, although there is a measure μ_b (the pure point measure) with

$$\delta_b(\varphi) = \int \varphi(x)\,d\mu_b(x)$$

but the symbolism of (V.2) is so suggestive that one often writes

$$\delta_b(\varphi) = \int \varphi(x)\delta(x-b)\,dx \tag{V.3}$$

$\delta(x-b)$ is not a function; (V.3) should be treated merely as a symbolic expression. $\delta(x-b)$ is called the **delta function at b.**

Example 4 (polynomially bounded measures) Suppose ν is any finite measure. Then $f \mapsto \int_{-\infty}^{\infty} f(x)\,d\nu$ is a linear functional on $\mathscr{S}$ and since $\left|\int f\,d\nu\right| \le \nu(\mathbb{R})\|f\|_\infty$ this functional is in $\mathscr{S}'$. In general, if ν is a measure on $\mathbb{R}$ so that $\nu([-D, D]) \le C(D^n + 1)$ for some C and n, and all $D \in \mathbb{R}_+$, then $f \mapsto \int_{-\infty}^{\infty} f\,d\nu$ is in $\mathscr{S}'$.

Example 5 (derivative of $\delta(x)$) To see that not every $g \in \mathscr{S}'$ comes from a linear combination of measures, consider $\delta'(f) = -f'(0)$. This is a continuous linear functional, but it does not comes from a measure (Problem 21).

Example 6 ($\mathscr{P}(1/x)$) The Cauchy principle part integral is given by

$$\mathscr{P}\left(\frac{1}{x}\right): f \mapsto \lim_{\varepsilon \downarrow 0} \int_{|x| \ge \varepsilon} \frac{1}{x} f(x)\,dx$$

To see that this is finite for any $f \in \mathscr{S}(\mathbb{R}^1)$ and is in fact a distribution, we note that

$$\int_{|x| \ge \varepsilon} \frac{1}{x} f(x)\,dx = \int_{\varepsilon}^{\infty} \frac{f(x) - f(-x)}{x}\,dx$$

Since $[f(x) - f(-x)]/x \to 2f'(0)$ as $x \to 0$, we can write

$$\mathscr{P}\left(\frac{1}{x}\right)(f) = \int_0^{\infty} \frac{f(x) - f(-x)}{x}\,dx$$

which proves it is finite. Since

$$\left|\frac{1}{x}[f(x) - f(-x)]\right| \le \frac{1}{x}\int_{-x}^{x} |f'(t)|\,dt \le 2\|f'\|_\infty$$

we have

$$\left|\mathscr{P}\left(\frac{1}{x}\right)(f)\right| \leq 2\int_0^1 \|f'\|_\infty \, dx + \left|\int_1^\infty (xf(x))\frac{dx}{x^2}\right|$$

$$\leq 2\|f\|_{1,0} + \|f\|_{0,1}$$

Thus $\mathscr{P}(1/x)$ is a distribution. The famous formula

$$\lim_{\varepsilon \downarrow 0} \frac{1}{x - x_0 + i\varepsilon} = \mathscr{P}\left(\frac{1}{x - x_0}\right) - i\pi\delta(x - x_0) \tag{V.4}$$

holds if all the objects are viewed as distributions and $\lim_{\varepsilon \downarrow 0}$ is interpreted in the $\sigma(\mathscr{S}', \mathscr{S})$ topology (Problem 22).

Example 7 (O_M^n) Let O_M^n denote the set of infinitely differentiable functions on $\mathbb{R}^n$ which together with their derivatives are polynomially bounded, that is, $f \in O_M$ means that f is C^∞ and for each $\alpha \in I_+^n$, there is an $N(\alpha)$ and a $C(\alpha)$ with

$$|(D^\alpha f)(x)| \leq C[1 + x^2]^N$$

where $x^2 = \sum_{i=1}^n x_i^2$. $O_M \subset \mathscr{S}'$.

The set O_M is useful for another reason. If $F \in O_M$, it is not hard to see that $Ff \in \mathscr{S}$ if $f \in \mathscr{S}$ and the map $f \mapsto Ff$ is a continuous map of $\mathscr{S} \to \mathscr{S}$ (Problem 23a). In fact, a measurable function F defines a continuous map $f \mapsto Ff$ of $\mathscr{S} \to \mathscr{S}$ if and only if $F \in O_M$ (Problem 23b).

Let $F \in O_M$. Then multiplication by F takes $\mathscr{S}$ into $\mathscr{S}$ continuously. This provides the first test of the philosophy expounded following Example 1. Can we find a map $S: \mathscr{S} \to \mathscr{S}$ so that for any $f, g \in \mathscr{S}$, $(Ff)(g) = (S'f)(g) = f(Sg)$, that is, so that $\int F(x)f(x)g(x)\,dx = \int f(x)(Sg(x))\,dx$. The answer is obvious: take $(Sg)(x) = F(x)g(x)$.

Operation 1 Let $F \in O_M^n$ and let $T \in \mathscr{S}'(\mathbb{R}^n)$. We define $FT \in \mathscr{S}'(\mathbb{R}^n)$ by

$$(FT)(\varphi) = T(F\varphi)$$

$\mathscr{S}$ was chosen partially to ensure that $f \to D^\alpha f$ would be continuous. Notice that $\|D^\alpha f\|_{\gamma,\delta} = \|f\|_{\gamma,\delta+\alpha}$ where $\delta + \alpha = \langle \delta_1 + \alpha_1, \ldots, \delta_n + \alpha_n \rangle$. To extend D^α to $\mathscr{S}'$ we seek $T: \mathscr{S} \to \mathscr{S}$ so that for $f, g \in \mathscr{S}$, $(D^\alpha f)(g) = f(Sg)$, that is, $\int (D^\alpha f)(x)g(x)\,dx = \int f(x)(Sg)(x)\,dx$. At first sight this appears difficult but integration by parts implies that $\int (D^\alpha f)g = (-1)^{|\alpha|}\int f(D^\alpha g)$ so we take $S = (-1)^{|\alpha|}D^\alpha$.

Operation 2 Let $T \in \mathscr{S}'(\mathbb{R}^n)$, $\alpha \in I_+^n$. The **weak derivative**, $D^\alpha T$, or **the derivative in the sense of distributions** is defined by

$$(D^\alpha T)(f) = (-1)^{|\alpha|} T(D^\alpha f)$$

In symbolic notation:

$$\int (D^\alpha T)(x) f(x)\, dx = (-1)^{|\alpha|} \int T(x) \left(\frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha}} f \right)(x)\, dx$$

We have thus defined a notion of derivative which coincides with the ordinary derivative on O_M^n and for which integration by parts without boundary terms at ∞ holds by fiat.

Example 8 Let

$$g(x) = \begin{cases} x, & x \geq 0 \\ 0, & x \leq 0 \end{cases} \qquad x \in \mathbb{R}$$

Then g is continuous but is not everywhere differentiable in the classical sense. Since $\int_{-\infty}^{\infty} g(x)\varphi(x)\, dx \leq \|x\varphi\|_{L^1}$, $g \in \mathscr{S}'$ so it has a derivative in $\mathscr{S}'$. By definition

$$\left(\frac{d}{dx} g\right)(\varphi) = -g\left(\frac{d\varphi}{dx}\right) = -\int_0^\infty x\varphi'(x)\, dx$$

$$= \int_0^\infty \varphi(x)\, dx$$

Thus $dg(x)/dx = H(x)$ where H is the **Heaviside function**

$$H(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}$$

H is not even continuous, but it too has a derivative in $\mathscr{S}'$ given by

$$\left(\frac{d}{dx} H\right)(\varphi) = -H\left(\frac{d\varphi}{dx}\right) = -\int_0^\infty \varphi'(x)\, dx = \varphi(0)$$

so $dH/dx = \delta$. δ, too has a derivative; it is described in Example 5.

This last example shows that even a nonfunction like δ is the second derivative of a continuous function. This is typical of tempered distributions, for

Theorem V.10 (regularity theorem for distributions) Let $T \in \mathscr{S}'(\mathbb{R}^n)$. Then $T = D^\beta g$ for some polynomially bounded continuous function g and some $\beta \in I_+^n$, that is,

$$T(\varphi) = \int (-1)^{|\beta|} g(x)(D^\beta \varphi)(x)\, d^n x$$

for all $\varphi \in \mathscr{S}$.

The proof is given in the appendix to this section (or see Problems 24 and 25).

Another operation is induced by translation. Let $U_a: \mathscr{S} \to \mathscr{S}$ by $(U_a f)(x) = f(x - a)$. Then $\int (U_a f)(x) g(x)\, dx = \int f(x)(U_{-a} g)(x)\, dx$ if $f, g \in \mathscr{S}$. Thus

Operation 3 (translation) $U_a T$ is defined for $T \in \mathscr{S}'$ by $(U_a T)(\varphi) = T(U_{-a}\varphi)$.

Similarly, if A is an invertible linear map of $\mathbb{R}^n \to \mathbb{R}^n$, we define $V(A): \mathscr{S} \to \mathscr{S}$ by $(V(A)f)(x) = f(A^{-1}x)$. Then, one has:

Operation 4 (linear coordinates changes) If $T \in \mathscr{S}'$, $V(A)T$ is given by

$$[V(A)T](\varphi) = |\det A|\, T(V(A^{-1})\varphi)$$

This extends $V(A)$ from $\mathscr{S}$ to $\mathscr{S}'$ (see Problem 28a).

In Chapter IX we discuss two other operations on $\mathscr{S}'$, convolution, and Fourier transform.

It is meaningless to say that a distribution vanishes at a point x, but vanishing in a neighborhood of x makes sense:

Definition Let Ω be an open set of $\mathbb{R}^n$. We say that $T \in \mathscr{S}'(\mathbb{R}^n)$ **vanishes in** Ω if $T(\varphi) = 0$ whenever φ has support in Ω (that is, whenever φ vanishes outside Ω). The **support of** T, supp T, is the complement of the largest open set on which T vanishes. If $T - S$ vanishes on Ω, we say $T = S$ on Ω.

These notions extend those of ordinary functions $\varphi \in \mathscr{S}$ (Problem 28b). Moreover, one has the following simple and intuitive result (Problem 29):

Theorem V.11 Let $T \in \mathscr{S}'(\mathbb{R}^n)$ and suppose that supp $T = \{0\}$. Then

$$T = \sum_{|\alpha| \le m} c_\alpha (D^\alpha \delta)$$

for suitable c_α and m.

Example 9 ($(1/x)_+$ renormalized) Consider the function $(1/x)_+ = H(x)x^{-1}$. Since $\int_0^1 (1/x)\,dx = \infty$, $(1/x)_+$ does *not* define a distribution. Let $\mathscr{S}(\mathbb{R}\backslash 0) = \{f \in \mathscr{S} \mid \operatorname{supp} f \in \mathbb{R}\backslash 0\}$. If $f \in \mathscr{S}(\mathbb{R}\backslash 0)$, $\int (1/x)_+ f(x)\,dx$ makes sense. Thus $(1/x)_+$ does define a linear functional on $\mathscr{S}(\mathbb{R}\backslash 0)$ which is continous as we shall see. By the Hahn–Banach theorem, this functional on $\mathscr{S}(\mathbb{R}\backslash 0)$ has extensions to all of $\mathscr{S}(\mathbb{R})$ which we call "renormalizations of $(1/x)_+$." As explicit examples, consider

$$\left(\frac{1}{x}\right)_{+,M}(f) = \int_0^M \frac{f(x) - f(0)}{x}\,dx + \int_M^\infty \frac{f(x)}{x}\,dx$$

Since these maps are continuous on $\mathscr{S}$, $(1/x)_+$ is continuous on $\mathscr{S}(\mathbb{R}\backslash 0)$. How much arbitrariness is there in the renormalization? If T and S are two renormalizations of $(1/x)_+$, then $T - S$ vanishes on $\mathscr{S}(\mathbb{R}\backslash 0)$ and so has support $\{0\}$; thus $T - S = \sum_{|\alpha| \le m} c_\alpha D^\alpha \delta$. For example,

$$\left(\frac{1}{x}\right)_{+,M} - \left(\frac{1}{x}\right)_{+,N} = -\ln\left(\frac{M}{N}\right)\delta(x)$$

With this definition of renormalization, there are an infinity of free constants in the renormalization of $(1/x)_+$. However, one could argue that as long as $f \in \mathscr{S}$ and $f(0) = 0$, $\int_0^\infty [f(x)/x]\,dx < \infty$; so we really want to extend $(1/x)_+$ from $\{f \in \mathscr{S} \mid f(0) = 0\}$ to $\mathscr{S}$. If we adopt this requirement, the only real renormalizations of $(1/x)_+$ are the $(1/x)_{+,M}$ and there is only one free constant in the renormalization (see Problem 32 for a link between these definitions).

Bogoliubov and Hepp have treated the renormalization of x space Feynman graphs in the spirit of Example 9; the renormalization constants, for example, the renormalized mass and charge, enter as the free constants analogous to the $\ln(M/N)$ in Example 9. For more details, see the references in the Notes.

There is one final theorem about $\mathscr{S}$ and $\mathscr{S}'$ which is often useful. To appreciate its significance, let us first consider the case of L^p where the analogous theorem fails. Suppose $p^{-1} + q^{-1} = 1$, $p < \infty$, $q < \infty$, and let $F \in L^q(\mathbb{R}^2) = [L^p(\mathbb{R} \times \mathbb{R})]^*$. Let $f, g \in L^p(\mathbb{R})$; then $f(x)g(y) \in L^p(\mathbb{R}^2)$ so

$$F(f, g) = \int F(x, y) f(x) g(y)\,dx\,dy < \infty$$

Moreover

$$|F(f, g)| \le \|F\|_{L^q(\mathbb{R}^2)} \|f\|_p \|g\|_p$$

so F defines a continuous bilinear form on L^p. Not every bilinear form is of this type. For example, if $p = 2$, the bilinear form $(f, g) = \int f(x)g(x)\,dx$

cannot be expressed as $(f, g) = \int F(x, y)f(x)g(y)\,dx\,dy$ for some $F \in L^2(\mathbb{R}^2)$.

The situation for $\mathscr{S}(\mathbb{R})$ and $\mathscr{S}(\mathbb{R} \times \mathbb{R})^* = \mathscr{S}'(\mathbb{R}^2)$ is very different:

Theorem V.12 (kernel or nuclear theorem) Let $B(f, g)$ be a separately continuous bilinear functional on $\mathscr{S}(\mathbb{R}^n) \times \mathscr{S}(\mathbb{R}^m)$. Then there is a unique tempered distribution $T \in \mathscr{S}'(\mathbb{R}^{n+m})$ with $B(f, g) = T(f \otimes g)$ where

$$(f \otimes g)(x_1, \ldots, x_{n+m}) = f(x_1, \ldots, x_n)g(x_{n+1}, \ldots, x_{n+m})$$

That separate continuity implies joint continuity is a consequence of the fact that $\mathscr{S}$ is Fréchet (Theorem V.9) and the corollary of Theorem V.7. We prove that jointly continuous functionals have the requisite form in the appendix to this section (Corollary 4 to Theorem V.14). Theorem V.12 can be extended to multilinear functionals (Problems 34 and 35).

Appendix to V.3 The N-representation for $\mathscr{S}$ and $\mathscr{S}'$

In this appendix, we will prove some of theorems about $\mathscr{S}$ and $\mathscr{S}'$. These proofs rely on the realization of $\mathscr{S}$ and therefore $\mathscr{S}'$ as sequence spaces (in fact as the space s of Section III.1). This realization depends in turn on two elements. The first element is topologizing $\mathscr{S}$ by an equivalent family of L^2 norms. To forcefully distinguish these norms from the $\|\cdot\|_{\alpha,\beta}$ norms we write

$$\|f\|_{\alpha,\beta,\infty} = \|x^\alpha D^\beta f\|_\infty$$

rather than merely $\|\cdot\|_{\alpha,\beta}$ and define

$$\|f\|_{\alpha,\beta,2} = \|x^\alpha D^\beta f\|_{L^2(\mathbb{R}^n)}$$

Then:

Lemma 1 The families of seminorms $\{\|\cdot\|_{\alpha,\beta,\infty}\}$ and $\{\|\cdot\|_{\alpha,\beta,2}\}$ on $\mathscr{S}(\mathbb{R}^n)$ are equivalent.

Proof We provide the proof in the case $n = 1$ for simplicity of notation. Since $(1 + x^2)^{-1} \in L^2$, $\|f\|_2 \leq \|(1 + x^2)^{-1}\|_2 \|(1 + x^2)f\|_\infty$ so

$$\|f\|_{\alpha,\beta,2} \leq C(\|f\|_{\alpha,\beta,\infty} + \|f\|_{\alpha+2,\beta,\infty})$$

On the other hand, $f(x) = \int_{-\infty}^{x} f'(x)\,dx$, so

$$\|f\|_\infty \le \|f'\|_1 \le \|(1+x^2)f'\|_2 \|(1+x^2)^{-1}\|_2$$

Since $(x^\alpha D^\beta f)' = \alpha x^{\alpha-1} D^\beta f + x^\alpha D^{\beta+1} f$ we have

$$\|f\|_{\alpha,\beta,\infty} \le C(\alpha\|f\|_{\alpha-1,\beta,2} + \|f\|_{\alpha,\beta+1,2} + \alpha\|f\|_{\alpha+1,\beta,2} + \|f\|_{\alpha+2,\beta+1,2}) \quad \blacksquare$$

The second element involves some special properties of Hermite functions (the eigenfunctions of the harmonic oscillator). Consider the maps $A: \mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R})$ and $A^\dagger: \mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R})$ given by

$$A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right) \qquad A^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)$$

and $N = A^\dagger A$. Let $\|f\|_n \equiv \|(N+1)^n f\|_2$ which is a seminorm on $\mathscr{S}$.

Lemma 2 The seminorms $\{\|\cdot\|_n\}$ are a directed family equivalent to the $\{\|\cdot\|_{\alpha,\beta,2}\}$ family of seminorms on $\mathscr{S}$.

Proof One need only use the inequality $\|A_1^* \cdots A_m^* f\|_2 \le \|(N+m)^{m/2} f\|_2$ where A^* stands for either A or $A^\dagger$. The details are left to the reader (Problem 36).

Now consider the function ϕ_0 defined by $A\phi_0 = 0$ and $\int_{-\infty}^{\infty} (\phi_0)^2\,dx = 1$, that is, $\phi_0(x) = \pi^{-\frac{1}{4}} e^{-\frac{1}{2}x^2}$ and let

$$\phi_n = (n!)^{-\frac{1}{2}}(A^\dagger)^n \phi_0 = (2^n n!)^{-\frac{1}{2}}(-1)^n \pi^{-\frac{1}{4}} e^{+\frac{1}{2}x^2}\left(\frac{d}{dx}\right)^n e^{-x^2}$$

The $\{\phi_n\}_{n=0}^\infty$ are called the **Hermite functions** or the harmonic oscillator wave functions since

$$\left(-\frac{d^2}{dx^2} + x^2\right)\phi_n = (2n+1)\phi_n$$

One has:

Lemma 3 The set $\{\phi_n\}_{n=0}^\infty$ is an orthonormal basis for $L^2(\mathbb{R})$.

Proof See Problems 6 and 7 of Chapter IX or Problems 30 and 31 of Chapter X.

Notice that $N\phi_n = n\phi_n$. Suppose $f \in \mathscr{S}$ and consider the L^2-convergent expansion $f = \sum_{n=0}^\infty a_n \phi_n$ where $a_n = (\phi_n, f) \equiv \int_{-\infty}^{\infty} \overline{\phi_n(x)} f(x)\,dx$. Since

$N^m: \mathscr{S} \to \mathscr{S}$, $N^m f \in \mathscr{S}$ and thus in L^2. But $N^m f = \sum_{n=0}^{\infty} a_n n^m \phi_n$, so $\sum_{n=0}^{\infty} |a_n|^2 n^{2m} < \infty$. In particular $\sup_n |a_n| n^m < \infty$. We have thus proven the first part of:

Theorem V.13 (the N-representation theorem for $\mathscr{S}$) Let s_k be the set of multisequences $\{a_\alpha\}_{\alpha \in I_+^k}$ with the property

$$\sup_{\alpha \in I_+^k} |a_\alpha| \, |\alpha|^m < \infty$$

for each m. Topologize s_k with the seminorms

$$\|\{a_\alpha\}\|_\beta^2 = \sum_\alpha (\alpha + 1)^{2\beta} |a_\alpha|^2$$

where $\beta \in I_+^k$ and $(\alpha + 1)^{2\beta} = \prod_{i=1}^k (\alpha_i + 1)^{2\beta_i}$. Let $f \in \mathscr{S}(\mathbb{R}^k)$. Then the sequence $\{a_\alpha\}$, $a_\alpha = (\phi_\alpha, f)$ with $\phi_\alpha(x) = \prod_{i=1}^k \phi_{\alpha_i}(x_i)$, is in s_k and the map $f \mapsto \{a_\alpha\}$ is a topological isomorphism. The **Hermite expansion** $f = \sum_\alpha a_\alpha \phi_\alpha$ converges in $\mathscr{S}$. The $\{a_\alpha\}$ are called **Hermite coefficients.**

Proof We give the details in the case $k = 1$. By our previous discussion, if $f \in \mathscr{S}$ and $a_n = (\phi_n, f)$, then $\{a_n\} \in s$. Moreover, $\|\{a_n\}\|_m = \|f\|_m$ in the notation of Lemma 2. Since the $\| \ \|_m$ are norms on $\mathscr{S}$, the map $f \mapsto \{a_n\}$ is injective. Now let $\{a_n\}_{n=0}^{\infty} \in s$ and let $f_N = \sum_{n=0}^{N} a_n \phi_n$. A simple computation shows that

$$\|f_N - f_M\|_m^2 = \sum_{n=N+1}^{M} |a_n|^2 (n+1)^{2m} \to 0$$

as $N, M \to \infty$. Thus f_N is Cauchy in each of $\| \ \|_m$ and thus in $\mathscr{S}$ (by Lemmas 1 and 2). Since $\mathscr{S}$ is complete, $f_N \to f$ for some $f \in \mathscr{S}$. But then $f_N \to f$ in L^2 so $(\phi_n, f) = a_n$. Thus the image of our map of $\mathscr{S} \to s$ is all of s. The equivalence of the topologies follows from the equality of the norms $\|\cdot\|_m$ on $\mathscr{S}$ and s. ∎

We can now identify $\mathscr{S}'$ with a sequence space also:

Theorem V.14 (the N-representation theorem for $\mathscr{S}'$) Let $T \in \mathscr{S}'(\mathbb{R}^k)$. Let $b_\alpha = T(\phi_\alpha)$ for each $\alpha \in I_+^k$. Then for some $\beta \in I_+^k$, $|b_\alpha| \leq C(\alpha + 1)^\beta$ for all α. Conversely, if $|b_\alpha| \leq C(\alpha + 1)^\beta$ for all α, there is a unique $T \in \mathscr{S}'$ with $T(\phi_\alpha) = b_\alpha$. If $T \in \mathscr{S}'$ and $b_\alpha = T(\phi_\alpha)$ are its **Hermite coefficients**, then $\sum_\alpha b_\alpha \phi_\alpha$ converges in the $\sigma(\mathscr{S}', \mathscr{S})$ topology to T.

Proof Again, we consider only $k = 1$. Let $T \in \mathscr{S}'$. Then $|T(\phi)| \leq C\|\phi\|_m$ for some m and C since $\{\|\cdot\|_m\}$ is a directed set. $\|\phi_n\|_m = (n+1)^m$, so

$|b_n| \le C(n+1)^m$. Conversely, suppose $|b_n| \le C(n+1)^m$. For $\{a_n\} \in s$ define $B(\{a_n\}) = \sum_{n=0}^{\infty} b_n a_n$. Then

$$|B(\{a_n\})| \le \sum_{n=0}^{\infty} |b_n||a_n| \le C \sum_{n=0}^{\infty} (n+1)^m |a_n|$$

$$\le C\left(\sum_{n=0}^{\infty} (n+1)^{2m+2}|a_n|^2\right)^{1/2}\left(\sum_{n=0}^{\infty}(n+1)^{-2}\right)^{1/2}$$

$$\le \frac{\pi^2}{6} C\|\{a_n\}\|_{m+1}$$

Thus B defines a continuous linear functional on s. Under the association of $\mathscr{S}$ and s, there is a $T \in \mathscr{S}'$ with $T(\sum_{n=0}^{\infty} a_n \phi_n) = \sum_{n=0}^{\infty} a_n b_n$; in particular, $T(\phi_n) = b_n$. The weak convergence of $\sum_n b_n \phi_n$ to T is easy. ∎

We can now easily prove many interesting theorems about $\mathscr{S}$ with this machinery which has *two* important simplifications: (1) Sequences are easier to deal with than functions. (2) The two conditions in $\mathscr{S}$, fall-off at ∞ and the C^∞ condition, are replaced by a *single* fall-off condition in s.

Corollary 1 $\mathscr{S}$ is dense in $\mathscr{S}'$ in the $\sigma(\mathscr{S}', \mathscr{S})$ topology.

Proof $\sum_{|\alpha| \le N} b_\alpha \phi_\alpha \in \mathscr{S}$ and converges weakly to $T \in \mathscr{S}'$ as $N \to \infty$ if $b_\alpha = T(\phi_\alpha)$. ∎

Corollary 2 $\mathscr{S}$ is separable in the Fréchet topology. $\mathscr{S}'$ is separable in the $\sigma(\mathscr{S}', \mathscr{S})$ topology (and also in the $\tau(\mathscr{S}', \mathscr{S})$ topology we introduce in Section V.7).

Corollary 3 The regularity theorem for distributions—Theorem V.10.

Proof Again we only consider the case $k = 1$. Since $\|f\|_\infty \le C\|(1+x^2)f'\|_2$ we conclude that $\|\phi_n\|_\infty \le C'(n+1)^{3/2}$, using A and $A^\dagger$ and the estimate in the proof of Lemma 2. (More detailed studies of the ϕ_n show $\|\phi_n\|_\infty \sim D(n+1)^{-1/12}$). Let $T \in \mathscr{S}'$ and let $\{b_n\}$ be its Hermite coefficients. Then $|b_n| \le E(n+1)^m$ for some m. Let $a_n = (n+1)^{-m-3}b_n$. Then $\sum |a_n| \, \|\phi_n\|_\infty \le E \sum (n+1)^{-3/2} < \infty$, so $\sum a_n \phi_n$ converges uniformly to some continuous function F on $\mathbb{R}$. F has Hermite coefficients (as an element of $\mathscr{S}'$), $\{a_n\}$. Extend $A^\dagger$, A and $N = \frac{1}{2}(-d^2/dx^2 + x^2 - 1)$ to $\mathscr{S}'$. Then

$$T = (N+1)^{m+3} F = \frac{1}{2^{m+3}}\left(-\frac{d^2}{dx^2} + x^2 + 1\right)^{m+3} F$$

Thus T can be written as a sum of polynomials times weak derivatives of polynomially bounded continuous functions. Simple manipulations (Problem 37) now complete the proof. ∎

Corollary 4 (nuclear theorem) Every jointly continuous bilinear functional $B(\cdot,\cdot)$ on $\mathcal{S}(\mathbb{R}^n) \times \mathcal{S}(\mathbb{R}^m)$ is of the form $B(f,g) = T(f \otimes g)$ for some $T \in \mathcal{S}'(\mathbb{R}^{n+m})$.

Proof Since B is jointly continuous, $|B(f,g)| \leq C\|f\|_r\|g\|_s$ for some $r \in I_+^n$, $s \in I_+^m$. Then $|B(\phi_\alpha, \phi_\beta)| \leq C(\alpha+1)^r(\beta+1)^s = C[\langle \alpha, \beta\rangle + 1]^{\langle r,s\rangle}$ where

$$\langle \alpha, \beta\rangle = \langle \alpha_1, \ldots, \alpha_n, \beta_1, \ldots, \beta_m\rangle \in I_+^{n+m}$$

As a result $b_{\langle\alpha,\beta\rangle} \equiv B(\phi_\alpha, \phi_\beta)$ are the Hermite coefficients of a distribution $T \in \mathcal{S}'(\mathbb{R}^{n+m})$ with $T(\phi_{\langle\alpha,\beta\rangle}) \equiv T(\phi_\alpha \otimes \phi_\beta) = b_{\langle\alpha,\beta\rangle}$. Let $f = \sum a_\alpha \phi_\alpha$, $g = \sum c_\beta \phi_\beta$. Since these expansions converge in $\mathcal{S}$,

$$T(f \otimes g) = \sum_{\alpha,\beta} a_\alpha c_\beta T(\phi_\alpha \otimes \phi_\beta) = \sum_{\alpha,\beta} a_\alpha c_\beta b_{\langle\alpha,\beta\rangle} = B(f,g) \quad ∎$$

V.4 Inductive limits: generalized functions and weak solutions of partial differential equations

In an intuitive sense, the distributions of the last section had the restriction of being polynomially bounded at infinity. We saw this in Theorem V.10 which told us any $T \in \mathcal{S}'$ is the derivative of a polynomially bounded function. The growth of a tempered distribution $T \in \mathcal{S}'$ is in some sense dual to the decrease restrictions imposed on functions $f \in \mathcal{S}$. This suggests we construct "distributions" without any growth restriction at ∞ as the dual of a space with the severest possible decrease conditions at ∞, that of vanishing outside of a compact set. That is, we want to topologize the C^∞ functions of compact support, $C_0^\infty(\mathbb{R}^n)$, so that it is a complete locally convex space. If K is a compact set in $\mathbb{R}^n$, the functions $C_0^\infty(K)$ which are C^∞ and have support in K have a natural topology given by $\|f\|_{\alpha,\infty} \equiv \sup_{\mathbb{R}^n} |D^\alpha f|$. $C_0^\infty(\mathbb{R}^n)$ is *not* complete when given the $\{\|\cdot\|_{\alpha,\infty}\}_{\alpha \in I_+^n}$ family of norms (see Problem 38), even though $C_0^\infty(K)$ is for each compact set K. In some sense, we want to think of $C_0^\infty(\mathbb{R}^n)$ as $\bigcup_m C_0^\infty(K_m)$ for some family of compact sets $\{K_m\}_{m=1}^\infty$ with $\bigcup_m K_m = \mathbb{R}^n$, and topologize it with a "limit" topology. To do this we describe a general construction.

Theorem V.15 Let X be a complex (or real) vector space. Let X_n be a family of subspaces with $X_n \subseteq X_{n+1}$, $X = \bigcup_{n=1}^{\infty} X_n$. Suppose that each X_n has a locally convex topology so that the restriction of the topology of X_{n+1} to X_n is the given topology on X_n. Let $\mathscr{U}$ be the collection of balanced, absorbing, convex sets $\mathcal{O}$ in X for which $\mathcal{O} \cap X_n$ is open in X_n for each n. Then:

(a) $\mathscr{U}$ is a neighborhood base at 0 for a locally convex topology.
(b) The topology generated by $\mathscr{U}$ is the strongest locally convex topology on X so that the injections $X_n \to X$ are continuous.
(c) The restriction of the topology on $\mathscr{K}$ to each X_n is the given topology on X_n.
(d) If each X_n is complete, so is X.

We require a technical lemma for the proof of Theorem V.15:

Lemma Let X be a locally convex space and let X_1 be a subspace with the relative topology (which is automatically locally convex). Let V be an open, convex, balanced subset of X_1. Then there is an open, convex, balanced set $Z \subset X$ so that $Z \cap X_1 = V$.

Proof Since X_1 has the relative topology we can find an open set $\mathcal{O} \subset X$ so $\mathcal{O} \cap X_1 = V$. Since $\mathcal{O}$ is a neighborhood of $0 \in X$ and X is locally compact, we can find $\mathcal{O}_1 \subset \mathcal{O}$ which is balanced, convex, and open in X. Let

$$Z = \{\alpha x + \beta y \mid x \in \mathcal{O}_1, \quad y \in V, \quad |\alpha| + |\beta| = 1\}$$
$$= \bigcup_{y \in V,\ |\alpha|+|\beta|=1,\ \alpha \neq 0} (\beta y + |\alpha| \mathcal{O}_1)$$

As a union of open sets, Z is open. Since $V \subset Z$, $V \subset (Z \cap X_1)$, but if $\alpha x + \beta y \in X_1 \cap Z$, then $x \in X_1 \cap \mathcal{O}_1 \subset X_1 \cap \mathcal{O} = V$ so $\alpha x + \beta y \in V$; that is, $Z \cap X_1 \subset V$. This proves the lemma. ∎

Proof of Theorem V.15 $\mathscr{U}$ is closed under finite intersections and dilatations, so we need only prove that the generated topology is Hausdorff to conclude (a). But if we can prove (c), it will follow that X is Hausdorff. For if $x \in X_n$ is given, we can find an X_n-open set $\mathcal{O}$ about $0 \in X_n$ with $x \notin \mathcal{O}$ and then, once (c) is proven, we can find U open in X with $U \cap X_n = \mathcal{O}$. Thus (c) implies (a). Given a neighborhood $\mathcal{O}_1$ of $0 \in X_n$ find a balanced, convex open set $N_n \subset \mathcal{O}_1$. Now, using the lemma, find $N_{n+1} \subset X_{n+1}$, convex, balanced, and open in N_{n+1}, so that $N_{n+1} \cap X_n = N_n$ and by induction, $N_k (k > n)$ so that N_k is convex, balanced, and open in X_k and $N_k \cap X_{k-1} = N_{k-1}$. Let $N_\infty = \bigcup_{k \geq n} N_k$. It is

easy to see $N_\infty \in \mathscr{U}$ and $N_\infty \cap X_k \subset \mathscr{O}_1$. Thus $\mathscr{O}_1$ is a neighborhood in the relative topology. That the relative topology is finer than the given topology follows from the definition of $\mathscr{U}$. This proves (c) and thus (a). (b) is easy. A reference for (d) is given in the notes. ∎

Definition The locally convex space X constructed in Theorem V.15 is called the **strict inductive limit** of the spaces X_n.

We remark that if each X_n is a proper closed subspace of X_{n+1}, then X is not metrizable (Problem 45). One of the nice properties of strict inductive limits is:

Theorem V.16 Let X be the strict inductive limit of the locally convex spaces $\{X_n\}_{n=1}^{\infty}$. Then a linear map T from X to a locally convex space Y is continuous if and only if each of the restrictions $T \restriction X_n$ is continuous.

Proof If T is continuous, each restriction is continuous. Conversely, suppose each restriction is continuous. Let N be a balanced, convex, open set in Y. Then $T^{-1}[N] \cap X_n = (T \restriction X_n)^{-1}[N]$ is open in X_n since $T \restriction X_n$ is continuous. Since $T^{-1}[N]$ is balanced and convex, it is open, so T is continuous. ∎

Example 1 Let $\kappa(\mathbb{R})$ be the continuous functions on $\mathbb{R}$ which have compact support. Let κ_n be those functions in $\kappa(\mathbb{R})$ with support in $[-n, n]$, normed with $\|\cdot\|_\infty$. Topologize κ with the inductive limit topology. By the last theorem, the dual of κ with this topology is precisely the complex Baire measures on $\mathbb{R}$. This construction works for $\kappa(X)$ when X is any σ-compact locally compact space.

Now let Ω be an open connected set in $\mathbb{R}^n$, $C_0^\infty(\Omega)$ the infinitely differentiable functions with compact support in Ω. Let K_n be an increasing family of compact sets with $\bigcup K_n^\circ = \Omega$. Put the Fréchet topology on $C_0^\infty(K_n)$ generated by the $\|D^\alpha f\|_\infty$ norms. The set $C_0^\infty(\Omega)$ with the inductive limit topology obtained by $C_0^\infty(\Omega) = \bigcup C_0^\infty(K_n)$ is denoted $\mathscr{D}_\Omega$. This topology is independent of the choice of the K_n (Problem 46). *Sequential* convergence in $\mathscr{D}_\Omega$ is fairly simple.

Theorem V.17 Suppose that $X = \bigcup X_n$ has a strict inductive limit topology and that each X_n is a closed proper subspace of X_{n+1}. Then a *sequence* $f_m \in X$ converges to $f \in X$ if and only if all the f_m are in some X_n

and $f_m \to f$ in the topology of that X_n. In particular, a *sequence* $f \in \mathscr{D}_{\mathbb{R}^n}$ converges to f if and only if all the f_m and f have support inside some fixed compact K and $D^\alpha f_m$ converges uniformly to $D^\alpha f$ for each multiindex α.

Proof Let $f_m \to f$ and suppose for all n, that there is an f_m with $f_m \notin X_n$. Then it is easy to construct subsequences of the f_m, say $g_i = f_{m(i)}$ and the X_n, say $Y_i = X_{n(i)}$ with $g_i \in Y_{i+1} \backslash Y_i$. Since Y_i is closed, we can use the Hahn–Banach theorem to find $\ell_i \in X^*$ so that $\ell_i \equiv 0$ on Y_i and $\ell_n(g_n) = n - \sum_{k=1}^{n-1} \ell_k(g_n)$. Let $\ell = \sum_{n=1}^{\infty} \ell_n$. On any X_n, this sum is effectively finite, so ℓ is continuous on each X_n, and hence, by Theorem V.16, on X. Since $g_m \to f$, and $\ell \in X^*$, $\ell(g_m)$ converges. But $\ell(g_m) = m$; this contradiction proves that all the f_m are in some X_n. ∎

We are now ready to define the distributions on Ω:

Definition A **generalized function (or distribution)** is a continuous linear functional on $\mathscr{D}_\Omega$. The space of all continuous linear functionals on $\mathscr{D}_\Omega$ is denoted by $\mathscr{D}'_\Omega$. $\mathscr{D}$ and $\mathscr{D}'$ will denote $\mathscr{D}_{\mathbb{R}^n}$ and $\mathscr{D}'_{\mathbb{R}^n}$ respectively.

Theorem V.16 translates directly into:

Corollary A linear functional T on $\mathscr{D}_{\mathbb{R}^n}$ is continuous if and only if for each compact $K \subset \mathbb{R}^n$, there is a constant C and an integer j so that

$$|T(\varphi)| \leq C \sum_{|\alpha| \leq j} \|D^\alpha \varphi\|_\infty$$

for all $\varphi \in C_0^\infty(K)$.

Example 2 Let f be an arbitrary continuous function on $\mathbb{R}^n$, and define $D^\alpha f \in \mathscr{D}'$ by:

$$(D^\alpha f)(\varphi) = (-1)^{|\alpha|} \int f(x)(D^\alpha \varphi)(x)\, dx$$

Then for each compact set K and $\varphi \in C^\infty K)$

$$|(D^\alpha f)(\varphi)| \leq C \|D^\alpha \varphi\|_\infty \sup_{x \in K} |f(x)|$$

so $D^\alpha f \in \mathscr{D}'_{\mathbb{R}^n}$. Thus $\mathscr{D}'_{\mathbb{R}^n}$ contains the weak derivatives of all continuous functions.

Example 3 Consider $\mathscr{D}$. Let $\delta^n(x-a)\colon \mathscr{D} \to \mathbb{C}$ by $\delta^n(x-a)(f) = D^n f(a)$. Then $\sum_{n=0}^{\infty} \delta^n(x-n) = T$ is in $\mathscr{D}'$. For let $\varphi \in C_0^\infty[-m, m]$. Then

$$|T(\varphi)| = \left| \sum_{n=0}^{m} (D^n \varphi)(n) \right| \leq \sum_{n=0}^{m} \|D^n \varphi\|_\infty$$

This last example shows that $\mathscr{D}'_{\mathbb{R}^n}$ contains distributions T which are *not* the αth derivative of any continuous function. Thus, there is no direct analogue of Theorem V.10 for $\mathscr{D}'$ but there is a local regularity theorem (Problem 26). There is also a nuclear theorem for $\mathscr{D}$ (see Problems 59, 60).

One can also carry operations from $\mathscr{D}$ to $\mathscr{D}'$ by the method used in Section V.3. Thus, for example, if $p(x_1, \ldots, x_n)$ is a polynomial of total degree k in n variables, $p(x_1, \ldots, x_n) = \sum_{|\alpha| \le k} a_\alpha x^\alpha$, the partial differential operator $p(D) = \sum_{|\alpha| \le k} a_\alpha D^\alpha$ extends to $\mathscr{D}'$ by the formula

$$(p(D)T)(\varphi) = T\left[\sum_{|\alpha| \le k} (-1)^{|\alpha|} D^\alpha (a_\alpha \varphi)\right] \tag{V.5}$$

Formula (V.5) may also be used if the a_α are x-dependent C^∞ functions.

The extension of partial differential operators to $\mathscr{D}'$ is particularly useful in the theory of partial differential equations. Let f be a continuous function. A k-times continuously differentiable function u (we write $u \in C^k$) for which $p(D)u = f$ is called a **strict solution**. If $T \in \mathscr{D}'$ and $p(D)T = f$ with $p(D)T$ defined by (V.5), then T is called a **weak solution** of the partial differential equation. The difference between strict and weak solutions is only smoothness, for:

Proposition If $u \in C^k$, then $p(D)u$ defined by (V.5) is equal to the classical value of $p(D)u$. In particular, if $u \in C^k$ and f is continuous, u is a weak solution of $p(D)u = f$ if and only if it is a strict solution.

Proof An elementary integration by parts. ∎

The following example shows that not every weak solution is a strict solution:

Example Let $f(x)$ be the characteristic function of $[0, 1]$. We will show that $u(x, t) = f(x - ct)$ is a weak solution of $u_{tt} - c^2 u_{xx} = 0$. Rather than use the definition (V.5) directly (which is a useful exercise), we make use of the fact that the operator $p(D)$ in (V.5) is continuous on $\mathscr{D}'$. Since $f \in L^1(\mathbb{R})$, we can find a sequence f_n in $\mathscr{D}_{\mathbb{R}}$ with $f_n \to f$ in $L^1(\mathbb{R})$. It is then easy to see that $u_n(x, t) = f_n(x - ct) \to u(x, t)$ in $\sigma(\mathscr{D}', \mathscr{D})$. But $p(D)u_n$ can be computed classically, that is,

$$\frac{\partial^2}{\partial t^2} u_n(x, t) = c^2 f_n''(x - ct) \qquad \frac{\partial^2}{dx^2} u_n(x, t) = f_n''(x - ct)$$

Thus

$$\frac{\partial^2}{\partial t^2} u_n - c^2 \frac{\partial^2}{\partial x^2} u_n = 0 \qquad \text{so} \qquad \frac{\partial^2}{\partial t^2} u - c^2 \frac{\partial^2}{\partial x^2} u = 0$$

In Problem 47, we discuss the notion of a distribution being only a function of $x - ct$ and prove that any such distribution T satisfies

$$\frac{\partial^2}{\partial t^2} T - c^2 \frac{\partial^2}{\partial x^2} T = 0$$

The concept of weak solution is particularly useful because it is often easy to prove weak solutions exist (see Section IX.5 for the constant coefficient case). In the case of elliptic equations (see Section IX.6), one can prove a regularity theorem which assures that under certain conditions, every weak solution is a strict solution. Combining these two techniques one concludes the existence of strong solutions for elliptic partial differential equations. Because of the phenomenon of the last example, the case of hyperbolic equations is not so easy.

V.5 Fixed point theorems †

We wish to consider the solution of equations of the form $x = Tx$ in a variety of types of applications. For example, an inhomogeneous integral equation $f(x) = g(x) + \int K(x, y) f(y)\, dy$ is of the form $f = Tf$ with $Tf = g + Kf$, an affine linear map. The famous "bootstrap" equations proposed in particle physics are of the forms $S = T(S)$ where S is the S matrix and T is a very complicated operator. A Lorentz invariance condition on vacuum expectation values takes the form

$$W_n(x_1, \ldots, x_n) = W_n(\Lambda x_1, \ldots, \Lambda x_n)$$

where Λ is a fixed Lorentz transformation.

We want to discuss a variety of existence theorems for such equations —so-called fixed point theorems—and in Section V.6 we discuss some applications. We study them here because several of them are stated quite naturally in the language of locally convex spaces. We first consider "nonlinear" theorems, that is, theorems that make no assumptions on the linearity of the map T involved, and then one simple theorem which employs linearity.

Definition Let $T: X \to X$ be a map on a set X. A point $x \in X$ for which $Tx = x$ is called a **fixed point** of T.

The first nonlinear theorem is very simple and is probably familiar to the reader:

† A supplement to this section begins on p. 363.

Definition Let $\langle S, \rho \rangle$ be a metric space. A map $T: S \to S$ for which $\rho(Tx, Ty) \leq \rho(x, y)$ is called a **contraction**. If there is a $K < 1$ for which $\rho(Tx, Ty) \leq K\rho(x, y)$, T is called a **strict contraction**.

Theorem V.18 (contraction mapping principle) A strict contraction on a complete metric space has a unique fixed point.

Proof First, let us prove uniqueness. If $Tx = x$, $Ty = y$, then $\rho(x, y) = \rho(Tx, Ty) \leq K\rho(x, y)$. Since $K < 1$ and $\rho(x, y) \geq 0$, we conclude $\rho(x, y) = 0$, i.e. $x = y$. To prove existence, we first note that T is automatically continuous since $\rho(x, y) < K^{-1}\varepsilon$ implies $\rho(Tx, Ty) < \varepsilon$. Now, let x_0 be arbitrary and let $T^n x_0 \equiv x_n$. We will show that $\{x_n\}$ is Cauchy.

$$\begin{aligned} \rho(x_n, x_{n+1}) = \rho(Tx_{n-1}, Tx_{n-2}) &\leq K\rho(x_{n-1}, x_{-2}) \\ &\leq K^2\rho(x_{n-2}, x_{n-3}) \\ &\cdots \leq K^{n-1}\rho(x_1, x_0) \end{aligned}$$

Thus if $n > m$,

$$\rho(x_n, x_m) \leq \sum_{j=m+1}^{n} \rho(x_j, x_{j-1}) \leq K^m(1 - K)^{-1}\rho(x_0, x_1) \to 0 \text{ as } m \to \infty$$

Thus $\{x_n\}$ is Cauchy, so $x_n \to x$ for some x. Since T is continuous, $Tx = \lim Tx_n = \lim x_{n+1} = x$ which proves the theorem. ∎

The second theorem is much more difficult to prove and we have no intention of proving it here (see the notes); it generalizes the Brouwer fixed-point theorem which says that a continuous map of the closed unit ball in $\mathbb{R}^n$ into itself has at least one fixed point, a theorem which is already quite deep.

Theorem V.19 (Leray–Schauder–Tychonoff theorem) Let C be a nonempty compact convex subset of a locally convex space X. Let $T: C \to C$ be a continuous map. Then T has a fixed point.

As preparation for our last general fixed point theorem, we will prove Theorem V.19 in one special case (see the lemma below).

Definition Let X and Y be vector spaces, C a convex subset of X. A map $T: C \to Y$ is called an **affine linear map** on C if

$$T(tx + (1 - t)y) = tTx + (1 - t)Ty$$

for all $x, y \in C$ and all $0 \leq t \leq 1$.

Unlike the case of linear functionals on subspaces, continuous affine functionals on convex sets may not have continuous extensions to all of X (Problem 49).

Lemma Let T be a continuous affine map of C into itself where C is a compact convex subset of a locally convex space X. Then T has a fixed point.

Proof Let

$$x_n = \frac{1}{n}\sum_{i=0}^{n-1} T^i x_0$$

where x_0 is picked in C. Since C is convex, each $x_n \in C$. Since C is compact, some subnet $x_{n(\alpha)}$ converges to a limit x. We wish to show $Tx = x$. By the Hahn–Banach theorem, it is enough to show $\ell(Tx) = \ell(x)$ for any $\ell \in X^*$. Since C is compact, $\sup_{x \in C} |\ell(x)| \equiv M_\ell < \infty$ for any fixed ℓ. Thus

$$|\ell(Tx_n - x_n)| = \left|\ell\left(\frac{1}{n}T^n x_0 - \frac{1}{n}x_0\right)\right| \leq \frac{2}{n}M_\ell \to 0 \qquad \text{as} \qquad n \to \infty$$

As a result $\ell(Tx - x) = \lim_\alpha \ell(Tx_{n(\alpha)} - x_{n(\alpha)}) = 0$. ∎

The last fixed-point theorem that we consider deals with a whole family of maps:

Definition A family of maps $\mathscr{F}$ from a set X to itself is said to possess a **common fixed point** if there is an $x \in X$ so that $Tx = x$ for all $T \in \mathscr{F}$.

Theorem V.20 (Markov–Kakutani theorem) Let $\mathscr{F}$ be a family of *commuting* continuous affine maps of C into itself where C is a compact convex subset of a locally convex space; that is, $TSx = STx$ for all $S, T \in \mathscr{F}$ and $x \in C$. Then $\mathscr{F}$ has a common fixed point.

Proof For each finite subset $F \subset \mathscr{F}$, let $f_F = \{x \in C \mid Tx = x \text{ for all } T \in F\}$. Since the T are all continuous, each f_F is closed and clearly $f_{F_1} \cap f_{F_2} = f_{F_1 \cup F_2}$. Thus, if we can show each f_F is nonempty, $\bigcap_F f_F \neq \varnothing$ by the f.i.p. criterion, so there is an x with $Tx = x$ for all $T \in \mathscr{F}$. Since the $T \in \mathscr{F}$ are affine linear each f_F is convex. $x \in f_F$ implies $Sx \in f_F$ for each $S \in \mathscr{F}$ because $T \in F$ implies $T(Sx) = S(Tx) = Sx$ when $Tx = x$. Since f_F is convex, compact, and $S: f_F \to f_F$, there is an $x \in f_F$ with $Sx = x$, that is, $f_{F \cup \{S\}} \neq \varnothing$ if $f_F \neq \varnothing$. By induction, each f_F is nonempty so $\bigcap_F f_F \neq \varnothing$. As remarked above, this implies $\mathscr{F}$ has a common fixed point. ∎

In Chapter XIV, we return to the special properties of compact, convex subsets of locally convex spaces; in particular, in Section XIV.6, we extend Theorem V.20 to a variety of noncommutative cases (see also Problem 50).

V.6 Applications of fixed point theorems

A. Ordinary differential equations

Let F be a continuous function from $\mathbb{R} \times \mathbb{R}^n$ to $\mathbb{R}^n$. We are interested in solving the differential equation $\dot{y} \equiv dy/dt = F(t, y)$ with initial conditions; i.e. given $y_0 \in \mathbb{R}^n$, we want to find a continuously differentiable function, $y(t)$, on $\mathbb{R}$ for which $y(0) = y_0$ and $\dot{y}(t) = F(t, y(t))$ for all $t \in \mathbb{R}$. We will discuss how the fixed point theorems of Section V.5 can be applied to prove the existence of *local* solutions, that is, given y_0, we will find δ and a function, $y(t)$ on $(-\delta, \delta)$ obeying $y(0) = 0$ and $\dot{y}(t) = F(t, y(t))$ for all $|t| < \delta$. We remark that a pth order equation $y^{(p)} = F(t, y, \dot{y}, \ldots, y^{(p-1)})$ on $\mathbb{R}^k$ can be translated into a first-order equation on $\mathbb{R}^{kp}$ by letting Y be the column vector

$$Y = \begin{pmatrix} y \\ \dot{y} \\ \vdots \\ y^{(p-1)} \end{pmatrix} \equiv \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix} \quad \text{and solving} \quad \dot{Y} = \begin{pmatrix} y_2 \\ y_3 \\ \vdots \\ F(t, y_1, \ldots, y_p) \end{pmatrix}$$

Differentiation makes functions less smooth—it cannot usually be defined as a map from a space to itself unless the space contains only C^∞ functions. Integration is a much smoother operation—it takes continuous functions on an interval into themselves. Therefore, it is useful to rewrite the differential equation in integral form:

$$y(t) = y_0 + \int_0^t F(s, y(s))\, ds \tag{V.6}$$

It is easy to see that a continuous function $y(t)$ on $(-\delta, \delta)$ obeys (V.6) if and only if it is a local solution of $\dot{y}(t) = F(t, y(t))$ with the initial condition $y(0) = y_0$.

Thus given y_0 and δ, we consider the map G: $C[-\delta, \delta] \to C[-\delta, \delta]$, on the continuous functions from $[-\delta, \delta]$ to $\mathbb{R}^n$, given by

$$[G(g)](t) = y_0 + \int_0^t F(s, g(s))\, ds$$

Solving (V.6) is equivalent to finding a fixed point of G!

Consider, first the case where F is Lipschitz continuous; that is, given y_0, there is a K, δ, and ε so that $\|y - y_0\| < \varepsilon$, $|t| < \delta$ implies $\|F(y, t) - F(z, t)\| \leq K\|y - z\|$ if $\|z - y_0\| < \varepsilon$. $\|\cdot\|$ denotes the Euclidean norm on $\mathbb{R}^n$. By shrinking δ we can be sure that

$$\delta \max_{\substack{|t|<\delta \\ \|y-y_0\|<\varepsilon}} \|F(t, y)\| < \varepsilon \qquad \text{and} \qquad \delta K < \tfrac{1}{2}$$

Now, let

$$S = \{g \in C[-\delta, \delta] \mid \|g(t) - y_0\| \leq \tfrac{1}{2}\varepsilon, \forall t \in (-\delta, \delta)\}.$$

S is a complete metric space under $\|\cdot\|_\infty$ and $\delta \max\|F(t, y)\| < \varepsilon$ implies that $G(g) \in S$ if $g \in S$. The conditions $\delta K < \frac{1}{2}$ and $\|F(y, t) - F(z, t)\| \leq K\|y - z\|$ imply $\|G(g_1) - G(g_2)\|_\infty < \frac{1}{2}\|g_1 - g_2\|_\infty$, if $g_1, g_2 \in S$. Thus G is a strict contraction on S, so there is a *unique* $g \in S$ which satisfies (V.6) by Theorem V.18. It is not hard to see that any solution of (V.6) must obey $\|g(t) - y_0\| \leq \frac{1}{2}\varepsilon$ for t small and so must agree with the unique solution in S when t is small. In this case, we thus prove local existence and uniqueness.

Now suppose F is merely continuous. Given y_0, pick δ so that

$$\max_{\substack{|t|<\delta \\ \|y-y_0\| \leq 1}} |F(t, y)| < \delta^{-1}$$

Let

$$C_0 = \{g \in C[-\delta, \delta] \mid \|g(t) - y_0\| \leq 1, \forall t \in (-\delta, \delta)\}$$

Then $G(g) \in C_0$, if $g \in C_0$. Actually, more can be said; let

$$C_1 = \{g \in C_0 \mid \|g(t) - g(s)\| \leq |t - s| \max_{\substack{|t|<\delta \\ \|y-y_0\| \leq 1}} |F(t, y)|, \forall t, s \in (-\delta, \delta)\}$$

Then $g \in C_0$ implies $G(g) \in C_1$. Thus G: $C_1 \to C_1$. G is continuous and C_1 is convex and compact by equicontinuity arguments. Thus G has a fixed point by Theorem V.19.

Notice that the second method gives existence of local solutions, but not uniqueness also. In fact, when F is continuous but not Lipschitz, uniqueness may not hold: for example, if $F(t, y) = 2\sqrt{y}$, the equation $\dot{y} = 2\sqrt{y}$, $y(0) = 0$, has the two solutions, $y(t) \equiv 0$ and $y(t) = t^2$, which differ in any neighborhood of $t = 0$. The compactness of C_1 depends on the finite dimensionality of $\mathbb{R}^n$ where the unit ball is compact. However, the contraction in the Lipschitz case does not use compactness and thus goes through immediately for ordinary differential equations for functions with values in a Banach space.

The question of when local solutions can be continued to global solutions is much touchier.

B. Haar measure on commutative compact groups

One can use the Markov–Kakutani theorem for an easy construction of an invariant measure on a compact abelian group. Let G be a compact topological space which is also an abelian group and suppose that all the group operations are continuous. We wish to construct a measure $\mu \in \mathcal{M}_{+,1}(G)$ so that $\int f\,d\mu = \int f_g\,d\mu$ for any $g \in G$ and $f \in C(G)$ where f_g is the translate of f: $f_g(h) = f(h-g)$. For any $\mu \in \mathcal{M}_{+,1}(G)$, let $T_g\mu$ be defined by $T_g\mu(f) = \mu(f_g)$. Then $T_g\colon \mathcal{M}_{+,1}(G) \to \mathcal{M}_{+,1}(G)$ and is continuous in the vague (weak-$*$) topology. $\mathcal{M}_{+,1}$ is convex and is compact by the Banach–Alaoglu theorem. The various T_g commute since G is abelian. They are affine, so Theorem V.20 implies the existence of a common fixed point μ_{Haar} with the desired invariance property. In this case the fixed point theorem implies existence; uniqueness must be proven by a distinct argument.

C. Bootstrap equations

Without going into details, either technical or physical, we will describe an application of the Leray–Schauder–Tychonoff theorem to proving the consistency of certain bootstrap schemes.

In order to describe the bootstrap idea, let us fall back on potential scattering where there are fewer complications. Consider the scattering of two equal mass particles. Since the total momentum $\mathbf{P}$ is conserved and we will suppose that all forces depend only on the relative position of the particles, we can describe the scattering in a coordinate frame where $\mathbf{P} = \mathbf{0}$ (see Figure V.2).

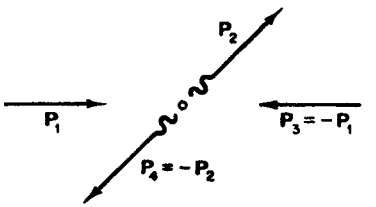

FIGURE V.2 Scattering when $\mathbf{P} = 0$.

For simplicity, we take $m = \frac{1}{2}$ where m is the mass of the particles. The natural variables in the nonrelativistic case are the energy $E = P_1^2 = P_2^2$ and the scattering angle θ, but for the proper relativistic correspondence, we take instead $s = 4E$ and the momentum transfer $t = -(\mathbf{P}_1 - \mathbf{P}_2)^2 = 2E(\cos\theta - 1)$.

In quantum mechanics, scattering is basically a wave phenomenon and is thus described by the magnitude of the scattered wave and its phase relative

to the incident wave; that is, by a complex number $A_{\text{phys}}(s, t)$, the scattering amplitude discussed in Section XI.6. It is defined in the region $E \geq 0$, $-1 \leq \cos\theta \leq 1$, or equivalently $0 \leq s < \infty$, $-s \leq t \leq 0$. As we shall see in Section XI.7, for a large variety of potentials the amplitude $A_{\text{phys}}(s, 0)$ is the boundary value of a function analytic in the cut s plane (Figure V.3). In

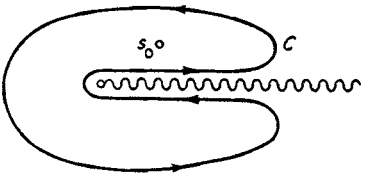

FIGURE V.3 The curve C in the cut s plane.

general there may be poles along the negative axis which we ignore for simplicity. Thus, $A_{\text{phys}}(s, 0) = \lim_{\varepsilon \downarrow 0} A(s + i\varepsilon, 0) \equiv A(s + i0, 0)$ for some analytic function in $\{s \mid \arg s \neq 0\}$. Moreover, $A(s, 0)$ is real for $s < 0$, so the Schwarz reflection principle implies that the physical amplitude obeys

$$\operatorname{Im} A(s + i0, 0) = \frac{1}{2i}[A(s + i0, 0) - A(s - i0, 0)]$$

Suppose, again for simplicity, that $A(s, 0) \to 0$ at infinity. In general, this is false and one must modify the argument below by what is known as making subtractions (see Section XI.7). Then, by the Cauchy integral theorem,

$$A(s_0, 0) = \frac{1}{2\pi i} \oint_C \frac{A(s, 0)}{s - s_0}\, ds$$

where C is the contour in Figure V.3. If we now make the large circle bigger and bigger, it will make no contribution since we assumed $A(s, 0) \to 0$ as $s \to \infty$. By shrinking the straight sections to the real axis, we find

$$A(s, t_0 = 0) = \frac{1}{\pi} \int_0^\infty \frac{D(s, t_0 = 0)}{s - s_0}\, ds \tag{V.7a}$$

where $D(s, t_0 = 0) = (1/2i)[A(s + i0, 0) - A(s - i0, 0)] = \operatorname{Im} A(s + i0, 0)$ is the "discontinuity" of A.

This "dispersion relation" (V.7a) can be proven to hold with $t = t_0$ for all real positive t_0 for a small class of potentials. This class includes sums of Yukawa potentials which are thought to be the nonrelativistic analogues of nuclear forces. Moreover, in that case, for s_0 fixed, $D(s_0, t)$ is the boundary value of an analytic function in a plane cut from $t = \sigma(s)$ to ∞. $\sigma(s)$ is a

function depending on the potential which is explicitly known and is called the Mandelstam boundary. We can write a dispersion relation for D

$$D(s, t_0) = \frac{1}{\pi} \int_{\sigma(s)}^{\infty} \frac{\rho(s, t)}{t - t_0} dt$$

where $\rho(s, t) = (2i)^{-1}[D(s, t + i0) - D(s, t - i0)]$ is called the "double spectral function."

Putting our two dispersion relations together, we obtain the "Mandelstam representation" for A

$$A(s, t) = \frac{1}{\pi^2} \int_0^{\infty} ds' \int_{\sigma(s')}^{\infty} dt' \frac{\rho(s', t')}{(s' - s)(t' - t)} \tag{V.7b}$$

This *linear* relation is essentially a statement of the analyticity properties of A.

The second element of the bootstrap scheme is the "unitarity of the S matrix." Let us temporarily revert to the (E, θ) variables and write $A(E, \theta)$ for the amplitude at $s = 4E$; $t = -2E(1 - \cos\theta)$. Unitarity is an expression of the fact that as many particles should leave the scattering region as enter it. Put differently, the number of particles scattered out of a beam must be the number lost from the beam (for a deeper discussion, see Section XI.4). Quantum mechanically, the decrease in the number of particles in the beam is due to interference between the scattered wave and the unscattered wave. This interference is proportional to Im $A(E, 0)$ while the amount scattered out of the beam is proportional to $|A|^2$. Thus, one finds the *nonlinear* relation

$$\text{Im } A(E, 0) = c \int |A(E, \theta)|^2 \, d\Omega$$

where $c(E)$ is a function of E dependent on normalization of A and $d\Omega$ is the angular measure on the sphere. One can extend this relation to nonzero θ and thus obtain a nonlinear integral relation between $D(s, t)$ and $A(s', t')$ (quadratic in A). By taking the discontinuity of D and using the Mandelstam representation for A one finds the relation

$$\rho = T(\rho)$$

where T is an explicit but complicated function of ρ. If ρ obeys $\rho = T(\rho)$ and has the proper decrease to make certain integrals converge, then one can show that A defined by (V.7b) obeys unitarity. Thus, the existence of $A(s, t)$ with the right analyticity and unitarity properties is equivalent to the existence of fixed points of T. Of course, in the nonrelativistic case, one knows that such ρ exist since one can show that the scattering amplitude for a superposition of Yukawa potentials has the right analyticity and unitarity properties.

In the relativistic case, for example, $\pi^0\pi^0$ scattering, there are two additional complications:

(*i*) *Crossing symmetry* Replace the momenta $\mathbf{p}_1, \mathbf{p}_2$ in Figure V.1 by the energy–momentum four-vectors $p_i = \langle \sqrt{\mu^2 + \mathbf{p}_i^2}, \mathbf{p}_i \rangle$ where μ is the mass of the pion. Given a four-vector $a = \langle a_0, \mathbf{a} \rangle$, we define $a^2 = a_0^2 - \mathbf{a}^2$; for example, $p_i^2 = \mu^2$, an expression of the relativistic energy–momentum relation. Now one defines the Mandelstam variables, $s = (p_1 + p_3)^2 = 4(p^2 + \mu^2)$ if p is the center of mass momentum, $t = (p_1 - p_2)^2 = \frac{1}{2}(s - 4\mu^2)(\cos\theta - 1)$ and $u = (p_1 - p_4)^2 = \frac{1}{2}(s - 4\mu^2)(-\cos\theta - 1)$. Of course, s, t, and u are not independent for $s + t + u = 4\mu^2$. Crossing symmetry expresses a deep fact of relativistic quantum theory, namely that the analytically continued amplitude for say $\pi^0\pi^0 \to \pi^0\pi^0$ is a symmetric function of s and t, and a symmetric function of s and u when the change of variables $\langle s, t \rangle \to \langle s, u \rangle$ is made by using $u = 4\mu^2 - s - t$. This automatically implies additional branch cuts in the domain of the function $A(s, t)$. For example, analogous to the cut in the domain of the nonrelativistic amplitude, running from $E = 0$ to $E = \infty$, is a cut in $A(s, 0)$ running from $s = 4\mu^2$ to $s = \infty$. Crossing symmetry implies that there must also be a cut running from $u = 4\mu^2$ to $u = \infty$, or equivalently, since $t = 0$, from $s = 0$ to $s = -\infty$. The analogue of nonrelativistic Mandelstam analyticity is then expressed by the relativistic Mandelstam relation

$$A(s_0, t_0) = \frac{1}{\pi^2} \int_{4\mu^2}^{\infty} ds \int_{\sigma(s)}^{\infty} dt\, \rho(s, t) \times \left[\frac{1}{(s - s_0)(t - t_0)} + \frac{1}{(s - s_0)(t + s_0 + t_0 - 4\mu^2)} + \frac{1}{(s + s_0 + t_0 - 4\mu^2)(t - t_0)} \right]$$

In this formula

$$\sigma(s) = \min\left\{ \frac{4s}{s - 16\mu^2}, \frac{16s}{s - 4\mu^2} \right\}$$

and ρ must obey $\rho(s, t) = \rho(t, s)$. The last two terms are just

$$\frac{\rho(s, u)}{(s - s_0)(u - u_0)} \quad \text{and} \quad \frac{\rho(t, u)}{(t - t_0)(u - u_0)}$$

after change of variable. This Mandelstam relation is just the expression of crossing symmetry plus certain analyticity properties.

(*ii*) *Inelastic processes* It is characteristic of relativistic systems that if there is sufficient energy available, large numbers of particles can be produced. For example if $s > 16\mu^2$, the reaction $\pi^0 + \pi^0 \to \pi^0 + \pi^0 + \pi^0 + \pi^0$ is

possible. Unitarity comes from a connection between the interference of the scattered and unscattered waves and the total amount scattered in *all* processes. It thus gives a relation between an $A(s, 0)$ and a sum of terms, one of which comes from $\pi^0 + \pi^0 \to \pi^0 + \pi^0$. Even when $4\mu^2 \leq \alpha \leq 16\mu^2$, an inelastic process $\pi^0 + \pi^0 \to \pi^+ + \pi^-$ is possible. A complete treatment would require consideration of all the $\pi + \pi \to \pi + \pi$ amplitudes. For simplicity we consider a model when there are no π^+ and π^-. Unitarity is thus a nonlinear equality on A only when $4\mu^2 \leq s \leq 16\mu^2$.

The "bootstrap hypothesis" of Chew and Mandelstam is the philosophical idea that there is only one set of amplitudes for all processes with the "usual" analyticity properties and which obey all the unitarity equations (coupling various processes). In practice, one approximates the equations, for example by replacing the coupled unitarity equations with inequalities when $s \geq 16\mu^2$ as we have done above. Whether one accepts the bootstrap philosophy or not, the various bootstrap equations are of interest since they can be viewed as an expression of the constraints placed by unitarity, crossing symmetry, and analyticity on the amplitude. Even if these do not determine the amplitude (and we do not subscribe to the bootstrap philosophy), they do put severe restrictions on the amplitude. In fact, it is not clear, a priori, that *any* functions $A(s, t)$ exist which obey the requisite analyticity *and* crossing symmetry, elastic unitarity if $4\mu \leq s \leq 16\mu^2$, and the unitarity inequalities for $16\mu^2 \leq s$.

The existence of such functions has been established by Atkinson in a beautiful application of the Leray–Schauder–Tychonoff theorem. The basic idea of the proof is the following. One seeks a function $\rho(s, t)$ to put into the Mandelstam representation. If A obeyed elastic unitarity everywhere, one would have

$$\rho(s, t) = (T^{\text{el}}\rho)(s, t)$$

where T^{el} is a complicated nonlinear map. Since elastic unitarity is only obeyed in certain regions, one has this equality only in certain regions of the s-t plane. In general $\rho(s, t) = (T^{\text{el}}\rho)(s, t) + v(s, t)$ where setting $v = 0$ in certain regions is equivalent to elastic unitarity. If v obeys certain other conditions, any solution of $\rho = T^{\text{el}}\rho + v$ obeying certain integrability conditions yields an A obeying elastic unitarity in $4\mu^2 \leq s \leq 16\mu^2$ and the inelastic unitarity inequalities in $s \geq 16\mu^2$. Thus, the existence of solutions of these approximate bootstrap equations would follow if $\rho = T\rho$ had a solution with $T\rho = T^{\text{el}}\rho + v$. What Atkinson does is to construct a convex set S_v, depending on v, of uniformly bounded, equicontinuous functions which is compact in the $\|\cdot\|_\infty$ topology and so that $T: S \to S$ and is continuous. The Leray–Schauder–Tychonoff theorem then provides the existence of solutions of of the approximate bootstrap equations.

D. Determining the phase of the scattering amplitude

According to quantum scattering theory (see Chapter XII), the "differential" scattering cross section at fixed energy is given by a function

$$D(\theta) = |F(\theta)|^2$$

where $F(\theta)$ is a complex-valued function of the scattering angle θ. At energies where there is only elastic scattering, F must obey the nonlinear "unitarity relation"

$$\operatorname{Im} F(\theta) = \int \overline{F(\theta_1)} F(\theta_2) \sin\theta_1 \, d\theta_1 \, d\varphi_1$$

where θ_2 is the function of θ_1, θ, and φ_1 determined by the spherical geometry in Figure V.4. $z_2 = \cos\theta_2$ is given in terms of $z = \cos\theta$, $z_1 = \cos\theta_1$, and φ_1 by

$$z_2 = zz_1 + (1 - z^2)^{1/2}(1 - z_1^2)^{1/2} \cos\varphi_1$$

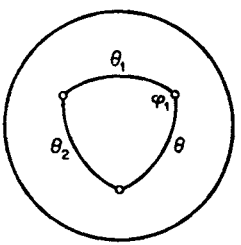

FIGURE V.4 The angle θ_2.

In experiments, one measures $D(\theta)$ while $F(\theta)$ is of great theoretical interest. There are two questions one immediately wants to ask: (1) Does the unitarity relation place any restrictions on the possible functions $D(\theta)$ which come from functions F obeying the unitarity relation. (2) Given $D(\theta)$, is F determined by the condition $|F(\theta)| = |D(\theta)|^{1/2}$ and the unitarity condition. The reader should realize by now that these questions are really the existence and uniqueness aspects of a single question.

Introduce the variables $z_i = \cos\theta_i$. Let $K(z_1, z_2; z)$ be the Jacobian of the transformation from $\langle z_1, \varphi_1\rangle$ to $\langle z_1, z_2\rangle$. Let $B(z) = |D(\theta)|^{1/2}$ be given and write the putative $F(\theta) = B(z)e^{i\varphi(z)}$. Then

$$\sin\varphi(z) = \int_{-1}^{1}\int_{-1}^{1} K(z_1, z_2; z) \frac{B(z_1)B(z_2)}{B(z)} e^{-i(\varphi(z_1) - \varphi(z_2))} \, dz_1 \, dz_2$$

or (V.8)

$$\varphi(z) = \sin^{-1}\left[\iint K(z_1, z_2; z) \frac{B(z_1)B(z_2)}{B(z)} \cos[\varphi(z_1) - \varphi(z_2)] \, dz_1 \, dz_2\right]$$

Let

$$M = \iint |K(z_1, z_2; z)| \frac{B(z_1)B(z_2)}{B(z)} dz_1\, dz_2$$

Suppose $M < 1$. Then for any continuous function $\varphi(z)$ on $[-1, 1]$ the function $\mathscr{F}\varphi$ given by

$$(\mathscr{F}\varphi)(z) = \sin^{-1}\left[\iint K(z_1, z_2; z)\frac{B(z_1)B(z_2)}{B(z)} \cos[\varphi(z_1) - \varphi(z_2)]\, dz_1\, dz_2\right]$$

is well defined. Question (1) has a positive answer if and only if $\mathscr{F}$ has a fixed point. (2) is related to uniqueness as follows: Let $\mu = \sin^{-1}(M)$. First note that if the branch of $\sin^{-1}$ with $-\pi/2 < \sin^{-1} x \leq \pi/2$ is chosen, $\mathscr{F}$ takes the functions φ on $[-1, 1]$ with $\|\varphi\|_\infty \leq \mu$ into themselves. Also, if φ satisfies (V.8), is continuous, and $|\varphi(0)| < \pi/2$, then $\|\varphi\|_\infty \leq \mu$. Finally, we remark that $\varphi(z)$ satisfies (V.8) if and only if $\tilde{\varphi}(z) = \pi - \varphi(z)$ satisfies (V.8). Thus $\mathscr{F}\varphi = \varphi$ has exactly two solutions if and only if there is only one solution with $|\varphi(z)| \leq \mu$ for all z.

If $M < 0.79$, Martin has shown that $\mathscr{F}$ is a contraction on

$$\{\varphi \mid \|\varphi\|_\infty \leq \mu;\ \varphi \text{ continuous}\}$$

with a suitable metric. This implies uniqueness and existence. For the general $M < 1$, existence (but not uniqueness) has been shown by an application of the Leray–Schauder–Tychonoff theorem.

E. Existence of correlation functions at low density

Finally we will briefly discuss the application of a very simple fixed-point theorem to statistical mechanics. The theorem is (Problem 51):

Theorem V.21 Let K be a linear map of a Banach space onto itself with $\|K\| < 1$. Then, for any g, $f = g + Kf$ has a *unique* solution $f = \sum_{n=0}^{\infty} K^n g$. Let K_m be a sequence of such maps so that $\|K_m - K\| \to 0$ and $\|K_m\| < 1$. If $g_m \to g$, $f_m = g_m + K_m f_m$ and $f = g + Kf$, then $f_m \to f$.

In equilibrium statistical mechanics, one introduces "correlation functions," $\rho(x_1), \rho_2(x_1, x_2), \ldots, \rho_n(x_1, \ldots, x_n), \ldots$. In the infinite volume limit, where the boundary effects stop playing a role, $\rho_n(x_1, \ldots, x_n)$ is the probability *density* for finding particles at $x_1, \ldots, x_n$. Thus, for example, $\rho_1(x)$ should be a constant equal to the density.

In a box Λ of finite size, elementary statistical mechanics gives an explicit formula for the correlation functions $\rho_n^{(\Lambda)}(x_1, \ldots, x_n; \beta, z)$ where $\beta = (kT)^{-1}$

spaces also has the Mackey topology (Problem 52a,d). In particular, the spaces $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{D}(\mathbb{R}^n)$ have the Mackey topology.

We return to the question of finding all dual $\langle X, Y\rangle$ topologies. A locally convex topology $\mathscr{T}$ on X is called a **dual-$\langle X, Y\rangle$** topology if the topological dual of $\langle X, \mathscr{T}\rangle$ is Y.

The basic duality theorem which identifies all dual topologies says:

Theorem V.22 (Mackey–Arens theorem) Let $\langle X, Y\rangle$ be a dual pair. A locally convex topology $\mathscr{T}$ on X is a dual-(X, Y) topology if and only if

$$\sigma(X, Y) \subseteq \mathscr{T} \subseteq \tau(X, Y)$$

Proof For the geometric proof, see the appendix to this section.

Thus the dual topologies are precisely those between the weak topology and the Mackey topology (inclusive).

We have seen how to recover the norm topology on a Banach space X in terms of the dual pair $\langle X, X^*\rangle$. How about the norm topology on X^*? It is not the $\tau(X^*, X)$ topology unless X is reflexive, for the $\tau(X^*, X)$ dual is X. Clearly, the norm topology on X^* is the topology of uniform convergence on the unit ball in X and so we need a locally convex notion that singles out sets contained inside balls. This need is met by the notion of bounded set. Before defining this notion, we note:

Theorem V.23 Let E be a locally convex space with dual F. The following are equivalent for a set $A \subset E$:

(a) For any neighborhood, U, of $0 \in E$, $A \subset nU = \{nx \mid x \in U\}$ for some n.

(b) The polar of A, A° (which we define in the appendix to this section), is absorbing.

(c) For any continuous seminorm ρ on E, $\sup_{x \in A} \rho(x) < \infty$.

(d) For any $\ell \in F$, $\sup_{x \in A} |\ell(x)| < \infty$.

Proof The equivalence of (a) and (c) and of (b) and (d) are essentially matters of definition. Theorem V.4 says that (c) implies (d). So suppose (d) holds and a continuous seminorm ρ is given. Let $K_\rho = \{x \in E \mid \rho(x) = 0\}$ and let E_ρ be the vector space E/K_ρ. Then ρ "lifts" to a norm on E_ρ. Let π be the canonical map of $E \to E_\rho$ and let $A_\rho = \pi[A]$. It is easy to see that

$\sup_{x \in A} \rho(x) < \infty$ if and only if $\sup_{x \in A_\rho} \rho(x) < \infty$. Let $\bar{E}_\rho$ be the completion of E_ρ. $\bar{E}_\rho$ is a Banach space. Let $\ell \in (E_\rho)^*$. Then $\ell \circ \pi \in E^*$ so

$$\sup_{x \in A} |\ell(x)| = \sup_{x \in A} |(\ell \circ \pi)(x)| < \infty$$

Thus by the Banach–Steinhaus principle, $\sup_{x \in A_\rho} \rho(x) < \infty$. ∎

Definition A set $A \subset E$, a locally convex space, is called **bounded** if and only if one, and hence all, of the conditions (a)–(d) of Theorem V.23 hold.

Condition (d) makes it clear that the notion of boundedness is the same in all $\langle E, F \rangle$-dual topologies and is thus a notion associated most naturally with a duality on E rather than a single topology on E.

Example 3 If X is a Banach space, $A \subset X$ is bounded if and only if $\sup_{x \in A} \|x\| < \infty$, which holds if and only if A is contained in some multiple of the unit ball. Thus for any bounded linear map on X,

$$\sup_{x \in A} \|Tx\| \leq C_A \|T\|$$

Example 4 Let X be a strict inductive limit of spaces X_n with X_n a proper closed subspace of X_{n+1}. If x_n is a sequence with $x_n \notin X_n$, by using the construction in the proof of Theorem V.17, we can find a linear functional, $\ell \in X^*$ with $\sup_n \ell(x_n) = \infty$. Thus any bounded set $A \subset X$ must actually be a bounded subset of some X_n. Thus, for example, $A \subset \mathcal{D}_\Omega$ is bounded if and only if: (i) there is a compact $K \subset \Omega$ so that $\operatorname{supp} f \subset K$ when $f \in A$; (ii) $\sup_{x \in A} \|D^\alpha f\|_\infty < \infty$ for any $\alpha \in I_+^n$.

The first example tells us how to generalize the norm topology on X^*:

Definition Let E be a locally convex space. Let F be its dual. The **strong topology**, $\beta(F, E)$ on F is the topology of uniform convergence on bounded subsets of E; that is, the topology generated by the seminorms $\{\rho_A | A \subset E \text{ is bounded}\}$ where $\rho_A(f) = \sup_{x \in A} |f(x)|$.

Any $\sigma(E, F)$-compact set C of E is bounded because the $f \in F$ are continuous functions on C. Thus the *strong topology $\beta(F, E)$ is stronger than the Mackey topology.*

We have found a topology $\beta(F, E)$ only dependent on the dual pair $\langle F, E \rangle$ so that the norm topology on X^* is the $\beta(X^*, X)$ topology when X is a

is the inverse temperature, $z = e^{\beta\mu}$ is the fugacity, and μ is the chemical potential. z is small when the density is low, i.e. when the system is a gas. One goal of classical statistical mechanics is to prove the existence of

$$\lim_{\Lambda \to \infty} \rho_n^{(\Lambda)}(x_1, \ldots, x_n, \beta, z)$$

at least for small z and/or β, i.e., for high temperature and/or low density where the system should be a gas, so there are no problems associated with the presence of several phases. This can be accomplished by the use of Theorem V.21. In a finite box, one shows that $\{\rho_n^{(\Lambda)}\}_{n=1}^{\infty}$ obeys a system of coupled integral equations (the Kirkwood–Salzburg equations):

$$\rho_1^{(\Lambda)}(x_1) = g_1^{(\Lambda)}(x_1) + \sum_{n=1}^{\infty} \int dy_1 \cdots dy_n K_{1,n}^{(\Lambda)}(x_1; y_1, \ldots, y_n)\, \rho_n^{(\Lambda)}(y_1, \ldots, y_n)$$

$$\rho_m^{(\Lambda)}(x_1, \ldots, x_m) = g_m^{(\Lambda)}(x_1, \ldots, x_m)\rho_{m-1}^{(\Lambda)}(x_2, \ldots, x_m)$$

$$+ \sum_{n=1}^{\infty} \int dy_1 \cdots dy_n K_{m,n}^{(\Lambda)}(x_1 \cdots x_m; y_1 \cdots y_n)$$

$$\times \rho_{n+m-1}^{(\Lambda)}(x_1, \ldots, x_m; y_1, \ldots, y_n)$$

Introducing a vector $\boldsymbol{\rho} = (\rho_1, \ldots, \rho_n, \ldots)$, these can be written schematically

$$\boldsymbol{\rho}^{(\Lambda)} = \mathbf{g}^{(\Lambda)} + \mathbf{K}^{(\Lambda)}\boldsymbol{\rho}^{(\Lambda)}$$

It turns out that one can introduce a norm on the set of $\boldsymbol{\rho}$ so that $\mathbf{K}^{(\Lambda)}$ is a bounded operator. For small z and/or β, one has $\mathbf{g}^{(\Lambda)} \to \mathbf{g}$ and $\mathbf{K}^{(\Lambda)} \to \mathbf{K}$ in the infinite volume limit, and all $\mathbf{K}^{(\Lambda)}$, $\mathbf{K}$ have norm less than one. By Theorem V.21, $\boldsymbol{\rho}^{(\Lambda)}$ converges in the limit of infinite volume to the unique solution of the infinite volume Kirkwood–Salzburg equations.

With regard to these last three examples, we caution the reader against thinking he has any real understanding of the technical details. We have tried to explain in a vague sense how fixed-point theorems arise—but all the hard work is in the choice of "suitable" norms or spaces and the proofs of bounds or continuity of maps. We have not considered these details at all.

V.7 Topologies on locally convex spaces: duality theory and the strong dual topology

In this section, we want to consider relations among various locally convex topologies on a vector space X. These topologies will not be used until Chapter XIV but their study develops useful intuition and illuminates the choice of topology on $\mathscr{S}$ and $\mathscr{D}$.

Let X be a vector space and Y a space of linear functionals on X which separates points; such a pair $\langle X, Y\rangle$ is called a **dual pair**. We already know that X has a locally convex topology, $\sigma(X, Y)$, in which the topological dual is precisely Y (Theorem IV.20). We first want to ask what other locally convex topologies on X produce Y as the topological dual.

Definition Let $\langle X, Y\rangle$ be a dual pair. The **Mackey topology** on X, $\tau(X, Y)$, is the topology of uniform convergence on $\sigma(Y, X)$-compact convex sets of Y; that is, $x_\alpha \xrightarrow{\tau(X,Y)} x$ if and only if $y(x_\alpha) \to y(x)$ uniformly as y runs through any fixed $\sigma(Y, X)$-compact convex subset of Y.

Alternatively, for each $\sigma(Y, X)$-compact convex subset C of Y, define the seminorm ρ_C on X by

$$\rho_C(x) = \sup_{y \in C} |y(x)|$$

The family of seminorms $\{\rho_C \mid C \text{ is } \sigma(Y, X)\text{-compact convex subset of } Y\}$ on X generates the $\tau(X, Y)$ topology. If C is compact, then

$$\tilde{C} = \{\lambda y \mid |\lambda| \leq 1, y \in C\}$$

is also compact (because $\{\lambda \mid |\lambda| \leq 1\}$ is compact) and $\rho_C = \rho_{\tilde{C}}$. Thus, we need only consider balanced, convex, $\sigma(Y, X)$-compact sets, C.

Since single points in Y are compact in the weak topology, if $x_\alpha \xrightarrow{\tau(X,Y)} x$, then $x_\alpha \xrightarrow{\sigma(X,Y)} x$, that is, the weak topology is weaker than the Mackey topology.

Example 1 Let X be a Banach space. Let X^* be its dual space. We claim that the $\tau(X, X^*)$ topology is just the norm topology on X. For the Banach–Alaoglu theorem (Theorem IV.21) tells us that the unit ball, X_1^*, in X^* is $\sigma(X^*, X)$ compact, so

$$\rho_{X_1^*}(x) = \sup_{y \in X_1^*} |y(x)|$$

is a Mackey seminorm. And, the Hahn–Banach theorem implies $\rho_{X_1^*}(\cdot) = \|\cdot\|_X$. On the other hand, if $C \subset X^*$ is $\sigma(X^*, X)$-compact, then for any $x \in X$, $y \mapsto y(x)$ is bounded on C so $C \subset \{y \mid \|y\| \leq m\}$ for some m by the Banach–Steinhaus principle. Thus $\rho_C(x) \leq m\|x\|_X$. This shows that the Mackey topology is generated by $\|\cdot\|_X$.

Example 2 We will see in Problem 52 that any Fréchet space, X, has the Mackey topology, $\tau(X, X^*)$. And, any *strict* inductive limit of Fréchet

Banach space. Given E, a locally convex space, we can form its dual E^* and put the $\beta(E^*, E)$ topology on it. The dual of E^* in this topology is called the **double dual** of E and is denoted by E^{**} when it is given the $\beta(E^{**}, E^*)$ topology. One can map E into E^{**} by the standard duality map, $\rho: E \to E^{**}$ by $\rho(x)(\ell) = \ell(x)$. This map is *not* always continuous (Problem 54). If it is a *topological* isomorphism, we say E is **reflexive**, that is, E is reflexive if:

(i) The $\beta(E^*, E)$ dual of E^* is E.
(ii) The $\beta(E, E^*)$ topology on E is the given topology.

The following criterion for reflexivity is often useful:

Lemma Let E be a locally convex space. Then E is reflexive if and only if all of the following hold:

(a) Every $\sigma(E, E^*)$-closed, bounded set of E is $\sigma(E, E^*)$ compact.
(b) Every $\sigma(E^*, E)$-closed, bounded set of E^* is $\sigma(E^*, E)$ compact.
(c) E has the Mackey (that is, $\tau(E, E^*)$) topology.

Proof It is not hard to see (Problem 55) that (a) holds if and only if the $\beta(E^*, E)$ and $\tau(E^*, E)$ topologies are identical and (b) says the $\beta(E, E^*)$ and $\tau(E, E^*)$ topologies are the same. Now, let E be reflexive. Since $E = E^{**}$, the $\beta(E^*, E)$ topology is a dual topology, so $\beta(E^*, E) \subset \tau(E^*, E)$ by the Mackey–Arens theorem. Since, $\tau \subset \beta$, $\beta(E^*, E) = \tau(E^*, E)$. Similarly, since the dual of E is E^* and E has the $\beta(E, E^*)$ topology, $\beta(E, E^*) = \tau(E, E^*)$ and E has the Mackey topology. Conversely, let (a)–(c) hold. By (a), $E = E^{**}$ as vector spaces since $\beta(E^*, E) = \tau(E^*, E)$ in that case, and the Mackey topology is a dual topology by Theorem V.22. By (b) and (c), E has the $\beta(E, E^*)$ topology. Thus E is reflexive. ∎

Using this lemma, one can prove (Problems 56, 57) that:

Theorem V.24 The spaces $\mathscr{S}(\mathbb{R}^n)$, $\mathscr{D}_\Omega$, and $\mathscr{O}_D$ are reflexive.

In general, the Mackey topology on a space is much stronger than the weak topology, so it is much harder for a set to be Mackey compact than weakly compact. For example, the unit ball in an infinite-dimensional Banach space is never norm compact (Problem 4) but it is weakly compact if X is reflexive. Thus general theorems on compactness in the Mackey topology are particularly strong statements. A most useful one is:

Theorem V.25 In $\mathscr{S}(\mathbb{R}^n)$, $\mathscr{D}_\Omega$, and $\mathscr{O}_D$, any closed bounded set is compact (in the usual Fréchet topology).

Proof Let $C \subset \mathscr{S}(\mathbb{R})$ be closed and bounded. Since $\sup_{f \in C} \|f'\|_\infty \equiv E < \infty$, $|f(x) - f(y)| \leq E|x - y|$ whenever $f \in C$. As a result, C is a uniformly equicontinuous family of uniformly bounded functions. Similarly,

$$\{x^\alpha D^\beta f \mid f \in C\}$$

are uniformly equicontinuous and uniformly bounded. By the Ascoli theorem and a diagonalization trick, any sequence in C has a convergent subsequence. Since C is closed and the topology is metric, this proves that C is compact. The proofs for $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{O}_D$ are similar. For $C \subset \mathscr{D}_\Omega$, we note that since C is bounded, $C \subset C^\infty(K)$ for some K and then use the above argument. ∎

A particularly useful consequence of this last theorem and Theorem V.8 is:

Theorem V.26 A *sequence* in $\mathscr{S}'$, $\mathscr{D}'$ or $\mathscr{O}'_D$ converges in the weak topology if and only if it converges in the strong topology.

Proof For $\mathscr{S}'$ and $\mathscr{O}'_D$ this follows directly from Theorems V.8 and Theorem V.25. In the case of $\mathscr{D}'$, we notice that any bounded set $C \subset \mathscr{D}$ lies in $C_0^\infty(K)$, which is a Fréchet space and then apply Theorem V.8 and Theorem V.25. ∎

Even though Theorem V.26 is essentially a corollary to Theorem V.25, we single it out as a theorem because it is very useful in applications. We caution the reader to heed the word *sequence*. The theorem does not hold if "net" replaces "sequence."

Appendix to V.7 Polars and the Mackey–Arens theorem

In this technical appendix, we prove the Mackey–Arens theorem by introducing the machinery of polar sets:

Definition Let $\langle E, F \rangle$ be a dual pair. Let $A \subset E$. The **polar of** A, A°, is $\{f \in F \mid |f(e)| \leq 1 \ \forall e \in A\}$. If we want F to be explicit, we write $(A)^\circ_F$.

Examples (1) Let $\mathscr{H}$ be a Hilbert space in duality with itself. If A is a subspace, $A^\circ \equiv A^\perp$.

(2) If E is a Banach space and F its dual,

$$\{x \mid \|x\|_E \leq k\}^\circ = \{y \mid \|y\|_F \leq k^{-1}\}$$

It is easy to prove the following simple properties of polar sets:

Lemma 1 Let $\langle E, F\rangle$ be a dual pair. Then

(a) A° is convex, balanced, and $\sigma(F, E)$ closed.
(b) If $A \subset B$, then $B^\circ \subset A^\circ$.
(c) If $\lambda \neq 0$, $(\lambda A)^\circ = |\lambda|^{-1} A^\circ$.
(d) $(\bigcup_\alpha A_\alpha)^\circ = \bigcap_\alpha A_\alpha^\circ$.

Polar sets are simply related to duals:

Theorem V.27 Let E be a locally convex space and $\mathscr{U}$ a neighborhood base at 0. Consider the dual pair, $\langle E, E^*_{\text{alg}}\rangle$, where E^*_{alg}, the algebraic dual, is the set of all linear maps of E into $\mathbb{C}$. Then the topological dual of E is $\bigcup_{U\in\mathscr{U}} U^\circ$ where the polars are taken relative to E^*_{alg}.

Proof $\ell \in E^*_{\text{alg}}$ is continuous if and only if $|\ell(x)| \leq 1$ for all x in some $U \in \mathscr{U}$, i.e. if and only if $\ell \in U^\circ$ for some $U \in \mathscr{U}$. ∎

Theorem V.28 (the bipolar theorem) Let E and F be a dual pair. Then using the $\sigma(E, F)$-topology on E, we have

$$E^{\circ\circ} = \overline{\text{a.c.h. } (E)}$$

where a.c.h.(E), the absolutely convex hull of E, is the smallest balanced convex set containing E, that is,

$$\text{a.c.h.}(E) = \left\{ \sum_{n=1}^{N} \alpha_n x_n \,\middle|\, x_1, \ldots, x_n \in E, \sum_{n=1}^{N} |\alpha_n| = 1, \quad N = 1, 2, \ldots \right\}$$

and the closure is in the $\sigma(E, F)$ topology.

Proof Let $E_C = \overline{\text{a.c.h.}(E)}$. Clearly $E \subset E^{\circ\circ}$ and since $(E^\circ)^\circ$ is convex, balanced, and $\sigma(E, F)$-closed, $E_C \subset (E^\circ)^\circ$. On the other hand, if $x \notin E_C$, we can find $\ell \in F$ with $\text{Re}\,\ell(e) \leq 1$ for $e \in E_C$ and $\text{Re}\,\ell(x) > 1$ (Theorem V.4). Since E_C is balanced, $\sup_{e\in E_C} |\ell(e)| \leq 1$ so $\ell \in E^\circ$. But then $|\ell(x)| > 1$ implies $x \notin E^{\circ\circ}$. ∎

Lemma 2 The Mackey topology is a dual topology.

Proof We use Theorem V.27 to compute the $\tau(E, F)$-dual of E. The $\{\rho_C\}$ as C runs through all $\sigma(F, E)$-compact, absolutely convex sets of F generate the $\tau(E, F)$-topology. Consider $C \subset F \subset E^*_{\text{alg}}$. Since the restriction of the $\sigma(E^*_{\text{alg}}, E)$ topology to F is $\sigma(F, E)$, C is $\sigma(E^*_{\text{alg}}, E)$-compact and so $\sigma(E^*_{\text{alg}}, E)$-

closed in E^*_{alg}. Thus, by Theorem V.28, $(C^\circ)^\circ_{E^*_{\text{alg}}} = C$. But $C^\circ = \{x \mid |\rho_C(x)| \leq 1\}$.The sets

$$\{C^\circ \mid C \text{ is a convex, balanced } \sigma(F, E)\text{-compact subset of } F\}$$

thus form a neighborhood base at $0 \in E$ for $\tau(E, F)$. Therefore,

$$E^*_\tau = \bigcup_C (C^\circ)^\circ_{E^*_{\text{alg}}} = \bigcup_C C = F \blacksquare$$

Lemma 3 (the Bourbaki–Alaoglu theorem) Let $U \subset E$ be a balanced, convex neighborhood of 0 in some $\langle E, F\rangle$ dual topology. Then U°_F is a $\sigma(F, E)$-compact set in F.

Proof This is essentially a restatement of the Banach–Alaoglu theorem (Theorem IV.21); see Problem 58.

Lemma 4 Every dual topology is weaker than the Mackey topology.

Proof Let ρ be a seminorm on E in some given dual topology. We will show that $\rho = \rho_C$ for some $\sigma(F, E)$-compact, convex subset, C, in F. Let $U = \{x \mid |\rho(x)| \leq 1\}$. Then U is balanced, convex and $\sigma(E, F)$-closed by an application of Theorem V.4 (see Problem 20c). Thus, $(U^\circ)^\circ = U$ by the double polar theorem. Let $C = U^\circ \subset F$. By Lemma 3, C is $\sigma(F, E)$-compact and it is convex. By definition $(U^\circ)^\circ = \{x \mid |\rho_C(x)| \leq 1\} = U$, so $\rho_C = \rho$. ∎

We are now ready for:

Proof of Theorem V.22 Since the $\sigma(E, F)$ and $\tau(E, F)$ topologies are dual topologies (Lemma 2 and Theorem IV.20) any $\mathscr{T}$ in between is also a dual topology. By definition, $\sigma(E, F)$ is the weakest possible dual topology and by Lemma 4, $\tau(E, F)$ is the strongest possible dual topology. ∎

NOTES

Section V.1 For general references on locally convex spaces, see: Choquet's book (ref. to Section IV.1); J. Kelley and I. Namioka, *Linear Topological Spaces*, Van Nostrand–Reinhold, Princeton, New Jersey, 1963; G. Köthe, *Topological Vector Spaces*, Springer–Verlag, Berlin and New York, 1969; A. and W. Robertson, *Topological Vector Spaces*, Cambridge Univ. Press, London and New York, 1964; H. Schaeffer, *Topological Vector Spaces*, Macmillan, New York, 1966.

The Robertsons' book is a delightful 154 page monograph, and of the remaining books we find the translation of Köthe's German classic the most readable. For those who like problems, the Kelley–Namioka book has many, but it is not as superb as Kelley's topology book.

The first formulation of the Hahn–Banach theorem in terms of separating convex sets is in S. Mazur, "Über konvexe Mengen in linearen normierten Räumen," *Studia Math.* **4** (1933), 70–84. The more modern form (Theorem V.4) is due to M. Eidelheit, "Zur Theorie der konvexen Mengen in linearen normierten Räumen," *Studia Math.* **6** (1936), 104–111, and S. Kakutani, "Ein Beweis der Satzes von M. Eidelheit über konvexe Mengen," *Proc. Imp. Acad. Tokyo* **13** (1937), 93–94.

Locally convex spaces are topological vector spaces in which the Hahn–Banach theorem holds and thus are spaces with large topological duals. The L^p spaces, $0 < p < 1$, serve as examples of spaces without any continuous linear functionals; see Köthe, pp. 156–158.

Section V.2 The term "Fréchet space" was coined by Banach in his classic book. Theorem V.5 is a special case of a general theorem on the metrizability of uniform spaces; see Kelley's *General Topology*, pp. 184–190.

Sections V.3 and V.4. The theory of general and tempered distributions was first formalized by L. Schwartz and is very well described in his classic: *Théorie des distributions*, Vols. I–II, Hermann, Paris, 1957, 1959. The five volumes by Gel'fand and co-workers, *Generalized Functions*, Academic Press, New York, 1964–1967, are also quite readable. Informally, many of the notions were already discussed by Bochner, Friedrichs, and Sobolev in the 1930s.

The treatment of renormalization of Feynman amplitudes mentioned in Section V.3 is discussed in N. N. Bogoliubov and O. S. Parasiuk, "Uber die Multiplikation der Kausalfunktionen in der Quantentheorie der Felder," *Acta. Math* **97** (1957), 227–266; K. Hepp, "Proof of the Bogoliubov–Parasiuk Theorem on Renormalization," *Commun. Math. Phys.* **2** (1966), 301–326; and E. Speer, *Generalized Feynman Amplitudes*, *Ann. Math.* Study #62.

The nuclear theorem (Theorem V.12) is the starting point of a general discussion of spaces in which such theorems hold. The theory of such nuclear spaces was first developed in A. Grothendieck: "Produits tensoriels topologiques et espaces nucléaires," *Mem. Amer. Math. Soc.* No. 16 (1955). See also Schaeffer (ref. to Section V.1), pp. 92–107, Gel'fand, Vol. 4, and F. Trèves, *Topological Vector Spaces, Distributions and Kernels*, Academic Press, New York, 1967.

The discussion in Appendix V.3 follows that in B. Simon, "Distributions and Their Hermite Expansions," *J. Math. Phys.* **12** (1971), 140–148. A representation of $\mathscr{S}$ by entire functions which also allows a proof of the nuclear theorem is discussed in the paper of V. Bargmann: "On a Hilbert Space of Analytic Functions and an Associated Integral Transform; II: A Family of Related Function Spaces. Application to Distribution Theory," *Comm. Pure App. Math.* **20** (1967), 1–102.

The notion of inductive limit was first discussed systematically by the French school of L. Schwartz, J. Dieudonné, and A. Grothendieck. There is a generalization of the notion of strict inductive limit which only requires that the injection $X_n \to X_{n+1}$ be continuous (rather than continuous and open). In addition, in defining this "inductive limit," the indexing set may be any directed set. For additional discussion, see Köthe, pp. 215–233, and Robertson and Robertson, pp. 76–100, 127–130. In particular, (d) of Theorem V.15 is proven in the Robertsons' book, p. 128.

For additional discussion of weak solutions of partial differential equations the reader may consult the following (listed in order of increasing sophistication required): I. Stakgold, *Boundary Value Problems of Mathematical Physics*, Vol. 1 and 2, Macmillan, New York, 1968; A. Friedman, *Partial Differential Equations*, Holt, New York, 1969; S. Agmon, *Lectures on Elliptic Boundary Value Problems*, Van Nostrand-Reinhold, Princeton, New Jersey, 1965; L. Hörmander, *Linear Partial Differential Operators*, Springer-Verlag, Berlin, 1963.

Section V.5 For a general discussion of fixed point theorems in nonlinear contexts, see T. L. Saaty and J. Bram, *Nonlinear Mathematics*, McGraw-Hill, New York, 1964, or M. A. Kransnosel'ski, *Topological Methods in the Theory of Nonlinear Integral Equations*, Pergamon, New York, 1964. Of particular interest are attempts to apply notions from algebraic topology to infinite dimensional spaces; see A. Granas, *Introduction to Topology of Function Spaces*, Univ. of Chicago Math. Notes, 1961, or J. Cronin, *Fixed Points and Topological Degree in Nonlinear Analysis*, Amer. Math. Soc., Providence, Rhode Island, 1964. The proof of Theorem V.19 may be found in N. Dunford and J. Schwartz, *Linear Operators*, Vol. I, pp. 453–457, Wiley (Interscience), 1957. The deepest part of the theorem relies on Brouwer's theorem on the closed unit ball—an "analytic proof" of the theorem can be found on pp. 468–470 of Dunford–Schwartz. For a more "natural" algebraic topological proof, see any text on homology theory, e.g. P. Hilton and S. Wylie, *Homology Theory*, Cambridge Univ. Press, London and New York.

That the Brouwer theorem extends to some infinite dimensional spaces was first noted by G. D. Birkoff and O. D. Kellogg, "Invariant Points in Function Space," *Trans. Amer. Math. Soc.* **23** (1922), 96–115. In two papers, J. Schauder, "Zur Theorie Stetiger Abbildungen in Funktionalräumen," *Math. Z.* **26** (1927), 47–65, 417–431; "Der Fixpunktsatz in Funktionalräumen," *Studia Math.* **2** (1930), 171–180, the case where X is a Banach space was proven. The general theorem was proved by A. Tychonoff, "Ein Fixpunktsatz," *Math. Ann.* **111** (1935), 767–776.

The Markov–Kakutani theorem was first proven in A. Markov, "Quelques théorèmes sur les ensembles abéliens," *Dokl. Akad. Nauk. SSSR* **10** (1936), 311–314, using Tychonoff's theorem on products of compact sets. The proof we give is that given by S. Kakutani, "Two Fixed-Point Theorems Concerning Bicompact Convex Sets," *Proc. Imp. Akad. Tokyo* **14** (1938), 242–245.

There is a rather large literature on additional fixed point theorems. For example E. Begle "A Fixed Point Theorem," *Ann. Math.* **51** (1950), 544–550; H. Bohenhwst and S. Karlin, "On a Theorem of Ville," in *Contributions to the Theory of Games* (H. W. Kuhn and A. W. Tucker, eds.), Princeton Univ. Press, Princeton, New Jersey, 1950; F. Browder, "Asymptotic Fixed Point Theorems," *Math. Ann.* **185** (1970), 38–61; S. Eilenberg and D. Montgomery, "Fixed Point Theorems for Multi-valued Transformations," *Amer. J. Math.* **68**, (1946), 214–222; K. Fan, "A Generalization of Tychonoff's Fixed Point Theorem," *Math. Ann.* **142** (1961), 305–310; I. Glicksberg, "A Further Generalization of the Kakutani Fixed Point theorem with Applications to Nash Equilibrium Points," *Proc. Amer. Math. Soc.* 3, (1952), 170–174; W. Horn, "Some Fixed Point Theorems for Compact Maps and Flows in Banach Spaces," *Trans. Amer. Math. Soc.* **149** (1970), 391–404; S. Kakutani, "A Generalization of Brouwer's Fixed Point Theorem," *Duke Math. J.* **8** (1941), 457–459; J. Leray, "Théorie des points fixés, indice total et nombre de Lefschetz," *Bull. Soc. Math. France* **87** (1959), 221–233; R. Nussbaum, "Some Fixed Point Theorems," *Bull. Amer. Math. Soc.* 77 (1971), 360–365.

Section V.6 For a discussion of the application of fixed point theorems to the theory of ordinary differential equations, see L. Loomis and S. Sternberg, *Advanced Calculus*, pp. 266–304, Addison-Wesley, Reading, Massachusetts, 1968, who also discuss an application of the contraction mapping theorem to differential calculus (pp. 166–167; 230–234), or C. Goffman, "Preliminaries to Functional Analysis," in *Studies in Modern Analysis*, (R. C. Buck, ed.), pp. 149–150, 153–154, Prentice Hall, Englewood Cliffs, New Jersey, 1962. Goffman gives a proof of our existence theorem employing equicontinuity and the Stone–Weierstrass theorem but avoiding the Leray–Schauder–Tychonoff theorem.

We discuss the Haar integral in more detail in Chapter XIV. For its history, see the notes to that chapter.

For a general discussion of the bootstrap philosophy, see G. Chew, *The Analytic S-Matrix*, Benjamin, New York, 1966.

The Mandelstam representation was first proposed by S. Mandelstam in "Determination of the Pion-Nuclear Scattering Amplitude from Dispersion Relations and Unitarity, General Theory," *Phys. Rev.* **112** (1958), 1344–1360. In potential scattering, it was first proven by R. Blankenbecker, M. L. Goldberger, N. N. Khuri, and S. A. Treiman, "Mandelstam Representation for Potential Scattering," *Ann. Phys.* **10** (1960), 62–93. For additional discussion of the potential scattering case, see V. de Alfaro and T. Regge, *Potential Scattering*, North–Holland Publ., Amsterdam, 1965.

The work of Atkinson which we discuss in Section V.6c can be found in D. Atkinson: "A Proof of the Existence of Functions that Satisfy Exactly Both Crossing and Unitarity," I, II, III, IV, *Nucl. Phys.* **B7** (1968), 375–408; **B8** (1968), 377–390; **B13** (1969), 415–436; **B23** (1970), 397–412. For additional discussion of fixed point theorems applied to integral equations in high energy physics, see C. Lovelace, "Uniqueness and Symmetry Breaking in *S*-Matrix Theory," *Commun. Math. Phys.* **4** (1967), 261–302; J. Kupsch, "Scattering Amplitudes that Satisfy a Mandelstam Representation with One Subtraction and Unitarity," *Nucl. Phys.* **B11** (1969), 573–587, or R. L. Warnock, "Nonlinear Analysis Applied to *S*-Matrix Theory," Boulder Lectures in Theoretical Physics, 1968. pp. 72–86, Benjamin, New York, 1969.

The work of Martin on determining the phase of the scattering amplitude from its magnitude and unitarity may be found in A. Martin, "Construction of the Scattering Amplitude from Differential Cross Sections," *Nuovo Cimento* **59A** (1969), 131–151. A discussion of the Martin results and some of the Atkinson bootstrap results using only the contraction mapping theorem may be found in D. Atkinson, "Introduction to the Use of Non-Linear Techniques in *S*-Matrix Theory," *Acta Phys. Austriaca Suppl.* **7** (1970), 32–70. The first person to use fixed point theorems to study the problem seems to be R. G. Newton in "Determination of the Amplitude from the Differential Cross Section by Unitarity," *J. Math. Phys.* **9** (1968), 2050–2055. Examples of differential cross sections with non-unique associated amplitudes (and $M > 1$ in the notation we use in Example (d)) are constructed in J. Crichton, "Phase-Shift Ambiguities for Spin-Independent Scattering," *Nuovo Cimento* **45A** (1966), 256–258.

Discussion of fixed-point theorems in statistical mechanics can be found in: D. Ruelle, *Statistical Mechanics*, pp. 72–86, Benjamin, New York, 1969; J. Groenveld, "Two Theorems on Classical Many-Particle Systems," *Phys. Lett.* **3** (1962), 50–51; O. Penrose, "Convergence of Fugacity Expansions for Fluids and Lattice Gases," *J. Math. Phys.* **4** (1963), 1312–1320; D. Ruelle, "Correlation Functions of Classical Gases," *Ann. Phys.* **25** (1963), 109–1230; and G. Gallavotti and S. Miracle-Sole, "Correlation Functions of a Lattice System," *Commun. Math. Phys.* **7** (1968), 274–288.

Section V.7 The notion of dual pair is due to J. Dieudonné and G. Mackey. The Mackey–Arens theorem was first proven by G. Mackey, "On Convex Topological Linear Spaces," *Trans. Amer. Math. Soc.* **60** (1946), 519–537, and by R. F. Arens, "Duality in Linear Spaces," *Duke Math. J.* **14** (1947), 787–794.

A space in which every closed convex, balanced, absorbing set is a neighborhood of zero is called *barrelled.* By the Baire theorem, every Fréchet space is barrelled and, by an elementary argument, any strict inductive limit of Fréchet spaces is barrelled. A barrelled space in which any closed bounded set is compact is called a *Montel* space. Thus Theorem V.25 says certain spaces are Montel spaces. Montel spaces are automatically reflexive (so Theorem V.24 follows from Theorem V.25) and their duals are also Montel spaces when given the Mackey (strong) topology. See Köthe, pp. 369–372 for details. In particular, $\mathscr{S}'$ and $\mathscr{D}'$ are also Montel spaces.

Often, the polar, A°, is defined to be $A^\circ = \{f \in F \mid \operatorname{Re} f(e) \geq -1 \text{ for all } e \in A\}$. If A is convex and balanced, this agrees with the definition we gave. When A is a cone, this new definition is much more useful. For example, with the definition in the text, the polar of $\{f \in C(X) \mid f \geq 0\}$ is $\{0\}$ while for the new definition, the polar is all positive measures.

PROBLEMS

1. (a) Prove that a locally convex space has a topology given by a single norm if the topology is generated by finitely many seminorms.
   (b) Prove that a locally convex space has a topology generated by a single norm if and only if 0 has a bounded neighborhood.

2. Let X be an infinite dimensional locally convex space and X^* its dual. Prove that no $\sigma(X, X^*)$-continuous semi-norm is actually a norm; so seminorms are essential.

3. (a) Let $\{\rho_\alpha\}_{\alpha \in A}$ be a family of seminorms so that some finite sum $\rho_{\alpha_1} + \cdots + \rho_{\alpha_n}$ is actually a norm. Prove that $\{\rho_\alpha\}_{\alpha \in A}$ is equivalent to a family of norms.
   (b) Prove that any locally convex topology on $\mathbb{R}^n$ is the usual topology. [Hint: Use the equivalence of all norms on $\mathbb{R}^n$ and the following construction: Pick a seminorm $\rho_1 \neq 0$ and let $V_1 = \{x \mid \rho_1(x) = 0\}$; $\dim V_1 \leq n-1$. If $V_1 \neq \{0\}$, pick $x_1 \in V_1$ and ρ_2 so $\rho_2(x_1) \neq 0$. Let $V_2 = \{x \mid (\rho_1 + \rho_2)(x) = 0\}$; $\dim V_2 \leq n-2$; etc.]
   (c) Let X be a locally convex space. Show that any linear functional on a finite dimensional subspace of X has a continuous extension to all of X.
   (d) Prove that any finite dimensional subspace of a locally convex space is closed.

4. The purpose of this exercise is to prove that every locally compact, locally convex space is finite dimensional.
   (a) Let U be a compact neighborhood of 0. Show that one can find $x_1, \ldots, x_n$ so that $U \subset \bigcup_{i=1}^n (x_i + \frac{1}{2}U)$ and thus a finite dimensional space, M, with $U \subset M + \frac{1}{2}U$.
   (b) Prove that $U \subset M + (\frac{1}{2})^m U$ for any m.
   (c) Prove that $U \subset \overline{M}$.
   (d) Conclude that $\overline{M} = X = M$.

5. Let X be a Banach space, X^* and X^{**} its dual and double dual. Let X_1 be the unit ball of X and X_1^{**} the unit ball in X^{**}. Prove that

(a) X_1 is $\sigma(X^{**}, X^*)$ dense in X_1^{**}. (Hint: Use theorem V.6(c) on X^* with the $\sigma(X^{**}, X^*)$ topology.)
(b) X is reflective if and only if its unit ball is $\sigma(X, X^*)$-compact.

†6. Prove the three propositions at the beginning of Section V.1.

†7. Prove that the families $\{\rho_C^{(2)}\}$ and $\{\rho_C\}$ on $\mathcal{O}_D$ are equivalent. (Hint: Use the Cauchy integral formula integrated over an annular region.)

†8. Let C be an absorbing subset of V with $tx \in C$ if $x \in C$ and $0 \leq t < 1$. Let ρ be the Minkowski functional for C. Prove that
(a) $\rho(tx) = t\rho(x)$ if $t \geq 0$.
(b) $\rho(x + y) \leq \rho(x) + \rho(y)$ if and only if for all $u, v \in C$ and $0 \leq t < 1$, $t(\frac{1}{2}u + \frac{1}{2}v) \in C$.
(c) $\rho(\lambda x) = |\lambda|\rho(x)$ if and only if for all $u \in C$ and λ with $|\lambda| < 1$, $\lambda u \in C$.
(d) $\{x|\rho(x) < 1\} \subset C \subset \{x|\rho(x) \leq 1\}$.

†9. Prove Theorem V.2.

†10. (a) Complete the proof of Theorem V.5.
(b) Prove the proposition following Theorem V.5.

11. Let A and B be absorbing sets with the property: If $x \in A$ (respectively B) and $0 \leq t \leq 1$, then $tx \in A$ (respectively B). Let ρ_A, ρ_B be their Minkowski functionals. Prove that
(a) $\rho_B \leq \rho_A$ if and only if $tA \subset B$ for all $0 \leq t < 1$.
(b) $\rho_{A \cap B} = \max(\rho_A, \rho_B)$.
(c) $\rho_{A \cup B} = \min(\rho_A, \rho_B)$.

12. In the theory of functions of several complex variables, one can have open sets $\mathcal{O}$, $\mathcal{O}'$ in $\mathbb{C}^n$ with $\mathcal{O} \subset \mathcal{O}'$, properly contained, but with the property that every function analytic in $\mathcal{O}$ has a continuation to $\mathcal{O}'$. In that case, let $K \subset \mathcal{O}$ be compact and let $\hat{K} = \{z \in \mathcal{O}' \mid |f(z)| \leq \sup_{w \in K}|f(w)|$ for all f analytic in $\mathcal{O}'\}$. It is a useful theorem in the theory that

$$\bigcup_{\substack{K \subset \mathcal{O} \\ \text{compact}}} \hat{K} = \mathcal{O}'$$

(a) Show that $\bigcup \hat{K} = \mathcal{O}'$ is implied by the equality of the topologies of uniform convergence on compact subsets of $\mathcal{O}$ and compacts of $\mathcal{O}'$.
(b) Use Theorem V.6 to prove the equality of topologies mentioned in (a).

13. Let Z be a metric space. Let X^* be the dual of a Fréchet space. Suppose that $f: Z \to X^*$ is continuous when X^* is given the $\sigma(X^*, X)$ topology. Prove that it is continuous when X^* is given the $\tau(X^*, X)$ topology. (Hint: Use Theorem V.8.)

14. If Z in Problem 13 is replaced with an arbitrary topological space, what happens to the conclusion?

15. The purpose of this problem is to prove that every uniformly convex Banach space (see Problem 25 of Chapter III for the definition of uniformly convex) is reflexive.
(a) Let X be uniformly convex and let $x, y \in X$, $\ell \in X^*$. Prove that, if $\|x\| = \|y\| = \|\ell\| = 1$, $\mathrm{Re}\,\ell(x) > 1 - \delta(\varepsilon)$ and $\mathrm{Re}\,\ell(y) > 1 - \delta(\varepsilon)$, then $\|x - y\| < \varepsilon$.
(b) Let X be uniformly convex, and suppose that $\{x_\alpha\}$ is a net in X so that $x_\alpha \to x \in X^{**}$ in the $\sigma(X^{**}, X^*)$ topology. Suppose that $\|x\| = 1$, $\|x_\alpha\| \leq 1$ for all α. Using (a), prove that x_α is $\|\cdot\|$-Cauchy.
(c) Prove that $X = X^{**}$. (Use Problem 5a.)

Remark: The theorem proven in Problem 15 is due to D. P. Milman, "On some criteria for the regularity of spaces of type (B)", *Dokl. Akad. Nauk SSSR* **20** (1938), 243–246, and B. J. Pettis, "A proof that every uniformly convex space is reflexive," *Duke Math. J.* **5** (1939), 249–253.

16. (a) Let $\varphi \in \mathscr{S}$ and let φ_y be the function in $\mathscr{S}$ defined by $\varphi_y(x) = \varphi(x - y)$. Prove that the map $y \to \varphi_y$ is a C^∞ function from $\mathbb{R}^n$ to $\mathscr{S}(\mathbb{R}^n)$ with $D^\alpha(\varphi_y) = (-1)^\alpha (D^\alpha \varphi)_y$. To say $y \to \varphi_y$ has derivative $\partial\varphi_y/\partial y_j$ as a function with values in $\mathscr{S}$ means

$$\lim_{y \to y_0} |y - y_0|^{-1} \left[\varphi_y - \varphi_{y_0} - \sum_{j=1}^{N} \frac{\partial}{\partial y_j} (\varphi_y) \cdot (y - y_0)_j \right] = 0$$

in the topology of $\mathscr{S}$.

(b) Let $T \in \mathscr{S}'$. Let $\varphi \in \mathscr{S}$. Define T^φ to be the function, $T^\varphi(y) = T(\varphi_y)$. Prove that $T^\varphi \in C^\infty$.

(c) Let $\varphi_n \in \mathscr{S}$ with $\varphi_n \to \delta$ in the weak topology on $\mathscr{S}'$. Prove that $T^{\varphi_n} \to T$ for all $T \in \mathscr{S}'$ in the weak topology on $\mathscr{S}'$.

(d) Prove that $\mathscr{S}$ is dense in $\mathscr{S}'$.

17. Let X and Y be locally convex spaces and let X^*, Y^* be their topological duals. Suppose that $T: X \to Y$ is linear and continuous. Define the adjoint T': $Y^* \to X^*$ by $[T'(y^*)](x) = y^*(Tx)$. Prove that

(a) If X^* and Y^* are given the $\sigma(X^*, X)$ and $\sigma(Y^*, Y)$ topology, then T' is continuous.

(b) If X and Y are given the $\sigma(X, X^*)$ and $\sigma(Y, Y^*)$ topology, then T is continuous.

(c) If X^* and Y^* are given the $\tau(X^*, X)$ and $\tau(Y^*, Y)$ topology, then T' is continuous. (Hint: use (b).)

(d) T takes bounded subsets of X into bounded subsets of Y.

(e) If X^* and Y^* are given the $\beta(X^*, X)$ and $\beta(Y^*, Y)$ topology, then T' is continuous.

18. Let $T: X \to Y$, locally convex spaces, with T linear and continuous. Put the weak topology on both X^* and Y^* so that $(X^*)^* = X$; $(Y^*)^* = Y$.

(a) Prove that $(T')' = T$ in this case.

(b) Conclude that T is continuous from X to Y when they are given the $\tau(X, X^*)$ and $\tau(Y, Y^*)$ topologies.

(c) Conclude that T is continuous from X to Y when they are given the $\beta(X, X^*)$ and $\beta(Y, Y^*)$ topologies.

19. Let $T: X \to Y$ locally convex spaces with T linear and continuous. Let T' be the adjoint map from $Y^* \to X^*$. Prove that

(a) T' is injective if and only if $\overline{\text{Ran } T} = Y$.

(b) $\overline{\text{Ran } T'} = X^*$ in the $\sigma(X^*, X)$ or $\tau(X^*, X)$ topology if and only if T is injective.

(c) Let $\iota: \mathscr{S} \to \mathscr{S}'$ be the natural map of $\mathscr{S}$ into $\mathscr{S}'$, then ι is continuous when $\mathscr{S}$ is given the $\sigma(\mathscr{S}, \mathscr{S}')$ topology and $\mathscr{S}'$ is given the $\sigma(\mathscr{S}', \mathscr{S})$ topology.

(d) Prove $\iota' = \iota$!

(e) Conclude $\iota(\mathscr{S})$ is dense in $\mathscr{S}'$ in the $\tau(\mathscr{S}', \mathscr{S})$ and the $\sigma(\mathscr{S}', \mathscr{S})$ topology.

20. Let X be a locally convex space, with dual X^*.

(a) Prove that any closed subspace in X is $\sigma(X, X^*)$ closed.

(b) Prove that all dual-$\langle X, Y \rangle$ topologies have the same closed subspaces.

(c) Let C be a closed convex subset of X. Prove that C is $\sigma(X, X^*)$ closed. (Hint: Use the separation theorem.)

(d) Prove that all dual-$\langle X, Y\rangle$ topologies have the same closed convex sets.
(e) Do all dual-(X, Y) topologies have the same compact convex sets?

†21. Prove directly that δ' (Example 5 of Section V.3) is in $\mathscr{S}'$. Prove that δ' does not come from a measure.

†22. (a) Prove that

$$\lim_{\varepsilon \downarrow 0} \frac{x - x_0}{(x - x_0)^2 + \varepsilon^2} = \mathscr{P}\left(\frac{1}{x - x_0}\right)$$

in the weak topology on $\mathscr{S}'$.
(b) Let φ_n be a sequence of bounded functions on $\mathbb{R}$ so that $\int_{|x-x_0|\geq\varepsilon} \varphi_n(x)\,dx \to 0$ as $n \to \infty$ for each $\varepsilon > 0$, $\varphi_n(x) \geq 0$, and $\int \varphi_n(x)\,dx = c$ independent of n. Prove that $\varphi_n \to c\delta(x - x_0)$ in the topology of $\mathscr{S}'$.
(c) Prove that

$$\lim_{\varepsilon \to 0} \frac{\varepsilon}{(x - x_0)^2 + \varepsilon^2} = \pi\delta(x - x_0)$$

(d) Prove formula (V.4).

†23. (a) Let $F \in O_M$. Prove that $f \to Ff$ is a bounded map of $\mathscr{S}$ into $\mathscr{S}$.
(b) Let F be a measurable function so that $Ff \in \mathscr{S}$ for all $f \in \mathscr{S}$. Prove that F is C^∞.
(c) If $f \to Ff$ is continuous, prove that $F \in O_M$.

24. Let $T \in \mathscr{S}'(\mathbb{R})$ with $|T(f)| \leq C\sum_{\alpha,\beta=0}^{n} \|x^\alpha(d/dx)^\beta f\|_\infty$. Map $\mathscr{S} \to C_n(\mathbb{R}) \oplus \cdots \oplus C_n(\mathbb{R})$ ($n + 1$ times) by $f \to \langle f, f', \ldots, f^{(n)}\rangle$ where $C_n(\mathbb{R})$ is the Banach space of continuous functions, f, with $\sup \|x^\alpha f\|_\infty < \infty$ for $\alpha = 1, \ldots, n$ with norm $\|f\|^{(n)} = \sum_{\alpha=0}^{n} \|x^\alpha f\|_\infty$. Use the Hahn–Banach and Riesz–Markov theorems to prove that T can be written

$$Tf = \sum_{\beta=0}^{n} \int D^\beta f\, d\mu_\beta$$

where $\mu_0, \ldots, \mu_n$ are complex measures of polynomial growth.

25. (a) Let μ be a polynomially bounded measure and let $F(x) = \int_0^x d\mu$; $G(x) = \int_0^x F(x)\,dx$. Prove that $\mu = G''$ in the sense of distributions.
(b) Prove the regularity theorem for $\mathscr{S}'(\mathbb{R})$ using Problems 24 and 25(a).

26. By mimicking Problems 24 and 25, prove the local regularity theorem for $\mathscr{D}'$: Given $T \in \mathscr{D}'(\mathbb{R}^n)$ and a compact set $C \subset \mathbb{R}^n$, there is a continuous function F on C and an α so that $Tf = (-1)^\alpha \int F(x)(D^\alpha f)(x)$ for all $f \in \mathscr{D}(\mathbb{R}^n)$ with $\operatorname{supp} f \subset C$.

27. Let U_a be translation by a as an operator on $\mathscr{S}'(\mathbb{R})$. Let d/dx be the derivative operation on $\mathscr{S}'$. Prove that $(U_a - 1)a^{-1}$ converges pointwise in the $\sigma(\mathscr{S}', \mathscr{S})$ topology to d/dx.

†28. (a) Prove that $V(A)$ defined by Operation 4 in Section V.3 agrees with $(V(A)\varphi)(x) = \varphi(A^{-1}x)$ if $\varphi \in \mathscr{S}$ is regarded as an element of $\mathscr{S}'$.
(b) Show that the support of a function $\varphi \in \mathscr{S}$ as a distribution is identical to $\overline{\{x \mid \varphi(x) \neq 0\}}$.

†29. (a) Let $\varphi \in \mathscr{S}(\mathbb{R}^n)$ with $\varphi(0) = 0$. Prove that there exist $\{\varphi_k\} \in \mathscr{S}$ with $0 \notin \operatorname{supp} \varphi_k$ for all k so that $\|x^\alpha(\varphi_k - \varphi)\|_\infty \to 0$ for all $\alpha \in I_+^n$.

(b) Let $\varphi \in \mathscr{S}(\mathbb{R}^n)$ with $(D^\beta\varphi)(0) = 0$ for all $\beta \in I_+^n$ with $|\beta| \leq m$. Prove that there are $\{\varphi_k\} \subset \mathscr{S}$ with $0 \notin \operatorname{supp} \varphi_k$ for all k so that $\|x^\alpha D^\beta(\varphi_k - \varphi)\|_\infty \to 0$ for all $\alpha \in I_+^n$ and β with $|\beta| \leq m$.

(c) Let $T \in \mathscr{S}'(\mathbb{R}^n)$ with

$$|T(f)| \leq C \sum_{\substack{|\beta| \leq m \\ |\alpha| \leq n}} \|x^\alpha D^\beta f\|_\infty$$

Suppose that $\operatorname{supp} T = \{0\}$ and let $\varphi \in \mathscr{S}$ with $D^\beta\varphi(0) = 0$ for $|\beta| \leq m$. Prove that $T(\varphi) = 0$.

(d) Let $T \in \mathscr{S}'(\mathbb{R}^n)$ obey

$$|T(\cdot)| \leq C \sum_{\substack{|\beta| \leq m \\ |\alpha| \leq n}} \|x^\alpha D^\beta \cdot\|_\infty$$

Let $\operatorname{supp} T = \{0\}$. Find constants $\{C_\beta\}_{|\beta| \leq m}$ so that

$$T(\psi) = \sum_{|\beta| \leq m} (-1)^\beta C_\beta (D^\beta\psi)(0)$$

for all $\psi \in \mathscr{S}$. Hint: Pick $\eta \in \mathscr{S}$, identically 1 near 0 and let

$$\varphi = \psi - \eta \sum_{|\beta| \leq m} \frac{x^\beta}{\beta!} (D^\beta\psi)(0)$$

(e) Prove Theorem V.11.

30. Let $F \in \mathscr{O}_M(\mathbb{R})$, $T \in \mathscr{S}'(\mathbb{R})$. Let $'$ denote the derivative on $\mathscr{S}'$. By manipulating the definitions of multiplication and $'$, prove $(FT)' = F'T + FT'$.

31. A map $S: \mathscr{S} \to \mathscr{S}$ is called **local** if $\operatorname{supp} S\varphi \subset \Omega$ whenever $\operatorname{supp} \varphi \subset \Omega$. A map $S: \mathscr{S}' \to \mathscr{S}'$ is called **local** if $\operatorname{supp} ST \subset \Omega$ whenever $\operatorname{supp} T \subset \Omega$.

(a) Let $S: \mathscr{S} \to \mathscr{S}$ be local. Prove that $S': \mathscr{S}' \to \mathscr{S}'$ is local.

(b) Which of the operations 1–4 are local?

*32. A distribution $T \in \mathscr{S}'$ is said to be of order at most n if

$$|T(\varphi)| \leq C \sum_{\substack{|\alpha| \leq k \\ |\beta| \leq n}} \|x^\alpha D^\beta \varphi\|$$

for some C and k. It is said to be of order at most n^- if for some fixed j and for any $D > 0$, there are k and C so that

$$|T(\varphi)| \leq D \sum_{\substack{|\alpha| \leq j \\ |\beta| = n}} \|x^\alpha D^\beta \varphi\| + C \sum_{\substack{|\alpha| \leq k \\ |\beta| \leq n-1}} \|x^\alpha D^\beta \varphi\|$$

We say T is of **order n**, if it is of order at most n, but not of order at most n^-. We say T is of **order n^-**, if it is of order at most n^- but not of order at most $n - 1$.

(a) Prove that the renormalizations $(1/x)_{+,M}$ of Example 9 are of order 1^-.

(b) Prove that any other renormalization of $(1/x)_+$ has order not less than 1.

*33. Prove that not every bilinear form on $L^p(\mathbb{R})$ $(1 < p < \infty)$ is of the form $F(f, g) = \int F(x, y) f(x) g(y)\, dx\, dy$ for some $F(x, y) \in L^q(\mathbb{R}^2)$.

[Hint: If $p \geq 2$, let $F(f,g) = \int G(x)f(x)g(x)\,dx$ for some $G \in L^r$; $1/r + 2/p = 1$; if $1 < p \leq 2$, let $F(f,g) = \int G(x-y)f(x)g(y)\,dx\,dy$ with $G \in L^r$, $1/r = 2(1-1/p)$.]

Remarks. 1) The $1 < p \leq 2$ example suggested in the hint requires Young's inequality which we prove in Section IX.4.
2) The nuclear theorem is true for $L^1(\mathbb{R})$, that is, every bilinear form on $L^1(\mathbb{R})$ is of the form $F(f,g) = \int F(x,y)f(x)g(y)\,dy$ for some $F \in L^\infty(\mathbb{R}^2)$. It is an interesting exercise to prove this from the Dunford–Pettis theorem which says: Let E be a separable Banach space, $T: E \to L^\infty(\mathbb{R})$. Then there is a measurable function g on $\mathbb{R}$ with values in E^* so that $\sup_{x \in \mathbb{R}} \|g(x)\| = \|T\|$ and $[T(e)](x) = [g(x)](e)$, a.e. x. For a proof of the Dunford-Pettis theorem, see Trèves, (ref. to Section V.3) pp. 469–473.

†*34.* Prove that a separately continuous multilinear form on $F_1 \times \cdots \times F_n$, is jointly continuous if all the F_i are Fréchet spaces.

†*35.* Extend the proof of the nuclear theorem in the appendix of V.3 to multilinear functionals; explicitly, if $B(f_1, \ldots, f_k)$ is a separately continuous k-linear functional on $\mathscr{S}(\mathbb{R}^{n_1}) \times \cdots \times \mathscr{S}(\mathbb{R}^{n_k})$, there is a $T \in \mathscr{S}'(\mathbb{R}^{n_1 + \cdots + n_k})$ with

$$B(f_1, \ldots, f_k) = T(f_1 \otimes \cdots \otimes f_k).$$

†*36.* Provide the details of the proof of Lemma 2 in the appendix to Section V.3.

†*37.* Complete the proof of Corollary 3 in the appendix to Section V.3.

38. Define $\mathscr{D}_{L^\infty}(\mathbb{R}^n) = \{f \mid f \text{ is a } C^\infty \text{ function on } \mathbb{R}^n \text{ with all its derivatives in } L^\infty(\mathbb{R}^n)\}$. Put the seminorms $\{\|\cdot\|_{\alpha,\infty}\}$ on $\mathscr{D}_{L^\infty}(\mathbb{R}^n)$, where $\|f\|_{\alpha,\infty} = \|D^\alpha f\|_\infty$.
(a) Prove that $\mathscr{D}_{L^\infty}$ is complete.
†(b) Prove that $C_0^\infty(\mathbb{R}^n)$ is not closed in $\mathscr{D}_{L^\infty}$ and find its closure.

39. Let $\mathscr{E}(\mathbb{R}^n) = \{f \mid f \text{ a } C^\infty \text{ function on } \mathbb{R}^n\}$. For any integer m and $\alpha \in I_+^n$, let

$$\|f\|_{(m),\alpha} = \sup_{|x| \leq m} |(D^\alpha f)(x)|$$

Norm $\mathscr{E}(\mathbb{R}^n)$ with $\{\|\cdot\|_{(m),\alpha} | \alpha \in I_+^n,\ m \in I_+\}$.
(a) Prove that $\mathscr{E}$ is complete.
(b) Prove that the natural injection, $\iota: \mathscr{D} \subset \mathscr{E}$ is continuous, so $\iota': \mathscr{E}' \subset \mathscr{D}'$ in a natural way.
(c) Prove that $T \in \mathscr{D}'$ is in $\mathscr{E}'$ if and only if T has compact support.

40. Prove that the natural map $\mathscr{D} \subset \mathscr{S}$ is continuous and conclude that $\mathscr{S}' \subset \mathscr{D}'$ in a natural way. Prove that $\mathscr{E}' \subset \mathscr{S}'$.

†*41.* Prove part (b) of Theorem V.15.

42. Extend Lemma 1 of the appendix to Section V.3 to prove that $\{\|\cdot\|_{\alpha,\beta,\infty}\}$ and $\{\|\cdot\|_{\alpha,\beta,p}\}$ are equivalent families for any fixed $1 \leq p < \infty$ if $\|f\|_{\alpha,\beta,p} = \|x^\alpha D^\beta f\|_{L^p(\mathbb{R}^n)}$.

43. *(a) Prove that s_m and s_n are isomorphic, that is, there is a continuous linear bijection with continuous inverse $T: s_m \to s_n$.
(b) Prove that $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{S}(\mathbb{R}^m)$ are topologically isomorphic.

44. Prove that the norms $\{\|\cdot\|_\beta\}$ and $\{\|\cdot\|_{\beta;p}\}$ on s_m are equivalent families if $\|a\|_{\beta;p}^p = \sum_\alpha (\alpha+1)^\beta |a_\alpha|^p$.

45. Let X be a strict inductive limit of X_n with each X_n a proper closed subspace of X. Suppose that $\{U_n\}$ is a countable decreasing family of neighborhoods of 0. Pick $x_n \in U_n \backslash X_n$.
(a) Prove that $\{x_n\}$ is not bounded.
(b) Show that $\{x_n\}$ would be bounded if U_n were a neighborhood base.
(c) Conclude X is not metrizable.

†*46.* (a) Suppose X is the strict inductive limit of spaces X_n. Suppose $\{Y_n\}$ is an increasing family of subspaces of X so that for any n, there is an N with $X_n \subset Y_N$. Prove that X is the strict inductive limit of the Y_n.
(b) Let $K \subset \Omega \subset \mathbb{R}^n$ with K compact and Ω open. Prove that if $\mathscr{D}_\Omega$ has a topology given by some family $\{K_n\}$, then the restriction of this topology to $C_0^\infty(K)$ is the one given by the $\|D^\alpha f\|_\infty$ norms.
(c) Prove that the topology on $\mathscr{D}_\Omega$ is independent of the choice of the increasing family K_n of compact sets.

†*47.* Let $y_1, \ldots, y_n$ be coordinates on $\mathbb{R}^n$. We say a distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ is **independent** of $y_{k+1}, \ldots, y_n$ or is a function of $y_1, \ldots, y_k$ if and only if for any translation

$$U_{a_{k+1},\ldots,a_n} : (y_1, \ldots, y_n) \to (y_1, \ldots, y_k, y_{k+1} + a_{k+1}, \ldots, y_n + a_n)$$
$$U_{a_{k+1},\ldots,a_n} T = T$$

(a) Let F be a measurable function on $\mathbb{R}^k$ which is locally L^1. Let T be the distribution associated with the function $F(y_1, \ldots, y_k)$ on $\mathbb{R}^n$. Prove that T is independent of $y_{k+1}, \ldots, y_n$.
(b) Let T be independent of $y_{k+1}, \ldots, y_n$. Prove that $(\partial T/\partial y_i) = 0$ if $i = k+1, \ldots, n$. [Hint: Look at Problem 27.]
(c) Let T be a distribution in $\mathscr{D}(\mathbb{R}^2)$ which is only a function of $x\text{-}ct = y_1$. Prove this notion is independent of what independent coordinate is taken for y_2.
(d) Let T be as in (c). Prove that $(\partial T/\partial t) = -c(\partial T/\partial x)$ and that $\partial T/\partial t$ is also a distribution which is only a function of $x\text{-}ct$.
(e) Conclude that

$$\frac{\partial^2}{\partial t^2} T - c^2 \frac{\partial^2}{\partial x^2} T = 0$$

48. Let T and S be commuting maps of a metric space into itself. Let $f_T = \{x \mid Tx = x\}$.
(a) Prove that $Sx \in f_T$ if $x \in f_T$.
(b) Suppose that T is a strict contraction. Prove that S has a fixed point.
(c) Let T^n be a strict contraction for some n. Prove that T has a unique fixed point.

†*49.* Let $X = \{\{x_n\} \in \ell_2 \mid |x_n| \leq 1/3^n\}$.
(a) Prove that X is a compact convex subset of l_2.
(b) Let f: $X \to \mathbb{C}$ be given by $f(x) = \sum_{n=1}^\infty 2^n x_n$. Prove that f is a continuous affine linear map on X.
(c) Prove that f has no continuous extension to all of ℓ_2.

50. Suppose that G is a group with an abelian subgroup N so that G/N is abelian (for example the family of rotations and translations of $\mathbb{R}^2$). Let C be a compact, convex subset of a locally convex space X. For each $g \in G$, let T_g, an affine linear map of C into C, be given so that $T_g T_h = T_{gh}$.
(a) Let $C_N = \{x \in C \mid T_n x = x \text{ for all } n \in N\}$. Prove that C_N is compact, convex, and nonempty.
(b) Suppose g_1, g_2 are in the same coset in G/N. Prove that $T_{g_1} \restriction C_N = T_{g_2} \restriction C_N$.
(c) Prove that there is $x \in C$ with $T_g x = x$ for all $g \in G$.

51. Prove Theorem V.21 directly.

52. A locally convex space X is called a **Mackey space** or a **bornological space** if for any locally convex space Y, any linear map T: $X \to Y$ which takes bounded sets into bounded sets is continuous.
(a) Let X be a Mackey space. Prove that it has the Mackey topology, $\tau(X, X^*)$. (Hint: Consider id: $X \to \langle X, \tau \rangle$.)
(b) Let $x_n \to 0$ in a metrizable locally convex space. Prove that there exists $\{\rho_n\} \in \mathbb{R}$ with $\rho_n \to \infty$ so $\rho_n x_n \to 0$. [Hint: Let U_n be a countable neighborhood basis, $U_{n+1} \subset U_n$. Pick n_k so $n \geq n_k$ implies $x_n \in (1/k)U_k$. Pick $\rho_n = k$ if $n_k \leq n < n_{k+1}$.]
(c) Prove that every metrizable locally convex space is a Mackey space. [Hint: Use (b) and the fact that a convergent sequence is bounded.]
(d) Prove that a strict inductive limit $X = \bigcup X_n$ with X_n a proper closed subspace of X_{n+1} is Mackey if each X_n is Mackey.
(e) Prove that a strict inductive limit of Fréchet spaces is a Mackey space.
(f) Conclude that the natural topologies on $\mathscr{S}$ and $\mathscr{D}$ are the Mackey topologies.

53. Let E be a locally convex space. Define the **natural topology** $\eta(E^{**}, E)$ on E^{**} as follows. Let $\mathscr{U}$ be the family of all balanced convex neighborhoods of $0 \in E$. For $U \in \mathscr{U}$, let $\tilde{U}$ be the E^{**} polar of $U^\circ \subset E^*$. The $\tilde{U}$ generate the natural topology. Prove:
(a) The natural topology is weaker than the $\beta(E^{**}, E^*)$ topology. (Hint: Every U° is bounded.)
(b) The restriction of the natural topology on E^{**} to E is the original topology on E, that is, ρ: $E \to \langle E^{**}, \eta \rangle$ is continuous and open.
(c) The *inverse* of the natural injection ρ: $E \to \langle E^{**}, \beta \rangle$ from Ran ρ to E is always continuous.

54. Let E be a Banach space with the *weak* topology. Prove that the injection ρ: $E \to \langle E^{**}, \beta \rangle$ is *never* continuous if E is infinite dimensional.

†*55.* Let $\langle E, F \rangle$ be a dual pair. Prove that every $\sigma(E, F)$-closed bounded set of E is $\sigma(E, F)$-compact if and only if the $\tau(F, E)$ and $\beta(F, E)$ topologies on F are identical.

**56.* (a) Let E be a Fréchet space. Prove that any $\sigma(E^*, E)$-closed bounded subset of E^* is $\sigma(E^*, E)$-compact. (Hint: Mimic the Banach–Alaoglu theorem, invoking the principle of uniform boundedness at the crucial place.)
(b) Prove the conclusion of (a) when E is a strict inductive limit of Fréchet spaces.

†*57.* Combine Problems 52 and 56 with Theorem V.25 to prove Theorem V.24.

†*58.* Prove Lemma 3 in the appendix to Section V.7.

59. Let $[-a, a] \subset \mathbb{R}$. Let $\varphi_n(x) = (2a)^{-1/2} \exp(\pi i n x/a)$; $n = 0, \pm 1, \pm 2, \ldots$. Given $f \in L^2[-a, a]$, let $a_n = (\varphi_n, f)$. Prove that $f \in L^2[-a, a]$ is in $\overline{C_0^\infty[-a, a]}$ if and only if $n^k a_n \to 0$ for all k(as $n \to \infty$). Develop norm inequalities to prove that s and $\overline{C_0^\infty[-a, a]}$ are isomorphic. Prove that the closure of $C_0^\infty[-a, a]$ is in $\mathscr{D}$.

60. (a) Let $B(\cdot, \cdot)$ be a bilinear functional on $C_0^\infty[-a, a]$ which is separately continuous. Prove that there is a $T \in C_0^\infty([-a, a] \times [-a, a])^*$ with $B(f, g) = T(f \otimes g)$ by mimicking the appendix to Section V.3 and using Problem 59.

(b) Let $B(\cdot, \cdot)$ be a bilinear functional on $\mathscr{D}_{\mathbb{R}}$, which is separately continuous. Prove that there is a $T \in \mathscr{D}'_{\mathbb{R}2}$ with $B(f, g) = T(f \otimes g)$.

61. Prove that $C_0^\infty(\mathbb{R})$ is nonempty, that is, construct an explicit function of compact support which is infinitely differentiable. Hint: First show that the function $f(x) = \chi_{(0,\infty)}(x) e^{-1/x}$ is C^∞ where $\chi_{(0,\infty)}$ is the characteristic function of $(0, \infty)$.

VI: Bounded Operators

I was at the mathematical school, where the master taught his pupils after a method scarce imaginable to us in Europe. The proposition and demonstration were fairly written on a thin wafer, with ink composed of a cephalic tincture. This the student was to swallow upon a fasting stomach, and for three days following eat nothing but bread and water. As the wafer digested the tincture mounted to the brain, bearing the proposition along with it.

Jonathan Swift in ***Gulliver's Travels***

VI.1 Topologies on bounded operators

We have already introduced $\mathscr{L}(X, Y)$, the Banach space of operators from one Banach space to another. In this chapter we will study $\mathscr{L}(X, Y)$ more closely. We emphasize the case which will arise most frequently later, namely, $\mathscr{L}(\mathscr{H}, \mathscr{H}) \equiv \mathscr{L}(\mathscr{H})$ where $\mathscr{H}$ is a separable Hilbert space. Theorem III.2 shows that $\mathscr{L}(X, Y)$ is a Banach space with the norm

$$\|T\| = \sup_{x \neq 0} \frac{\|Tx\|_Y}{\|x\|_X}$$

The induced topology on $\mathscr{L}(X, Y)$ is called the **uniform operator topology** (or **norm** topology). In this topology the map $\langle A, B \rangle \to BA$ of $\mathscr{L}(X, Y) \times \mathscr{L}(Y, Z) \to \mathscr{L}(X, Z)$ is jointly continuous.

We now introduce two new topologies on $\mathscr{L}(X, Y)$, the weak and strong operator topologies. There are other interesting and useful topologies on $\mathscr{L}(X, Y)$, but we delay their introduction until we need them in a later volume (see however the discussion at the end of Section 6 and the Notes).

The **strong operator topology** is the weakest topology on $\mathscr{L}(X, Y)$ such that the maps

$$E_x : \mathscr{L}(X, Y) \to Y$$

given by $E_x(T) = Tx$ are continuous for all $x \in X$. A neighborhood basis at the origin is given by sets of the form

$$\{S \mid S \in \mathscr{L}(X, Y), \quad \|Sx_i\|_Y < \varepsilon, \quad i = 1, \ldots, n\}$$

where $\{x_i\}_{i=1}^n$ is a finite collection of elements of X and ε is positive. In this topology a net $\{T_\alpha\}$ of operators converges to an operator T (written $T_\alpha \xrightarrow{s} T$) if and only if $\|T_\alpha x - Tx\| \to 0$ for all $x \in X$. The map $\langle A, B\rangle \to AB$ is separately but not jointly continuous if X, Y, and Z are infinite dimensional (see Problem 6a, b). We sometimes denote strong limits by the symbol s-lim.

The **weak operator topology** on $\mathscr{L}(X, Y)$ is the weakest topology such that the maps

$$E_{x,\ell}: \mathscr{L}(X, Y) \to \mathbb{C}$$

given by $E_{x,\ell}(T) = \ell(Tx)$ are all continuous for all $x \in X, \ell \in Y^*$. A basis at the origin is given by sets of the form

$$\{S \mid S \in \mathscr{L}(X, Y), \quad |\ell_i(Tx_j)| < \varepsilon, \quad i = 1, \ldots, n, \quad j = 1, \ldots, m\}$$

where $\{x_i\}_{i=1}^n$ and $\{\ell_j\}_{j=1}^m$ are finite families of elements of X and Y^* respectively. A net of operators $\{T_\alpha\}$ converges to an operator T in the weak operator topology (written $T_\alpha \xrightarrow{w} T$) if and only if $|\ell(T_\alpha x) - \ell(Tx)| \to 0$ for each $\ell \in Y^*$ and $x \in X$. Notice that in the case $\mathscr{L}(\mathscr{H})$, $T_\gamma \to T$ weakly just means that the "matrix elements" $(y, T_\gamma x)$ converge to (y, Tx). In the weak topology the map $\langle A, B\rangle \to AB$ is separately, but not jointly continuous if X, Y, and Z are infinite dimensional (see Problem 6c).

Remark The reader should not confuse the weak operator topology on $\mathscr{L}(X, Y)$ with the weak (Banach space) topology on $\mathscr{L}(X, Y)$. The former is the weakest topology such that the bounded linear functionals on $\mathscr{L}(X, Y)$ of the form $\ell(\cdot x)$ are continuous for all $x \in X$ and $\ell \in Y^*$. The latter is the weakest topology such that *all* bounded linear functionals on $\mathscr{L}(X, Y)$ are continuous (see Section VI.6).

Notice that the weak operator topology is weaker than the strong operator topology which is weaker than the uniform operator topology. In general, the weak and strong operator topologies on $\mathscr{L}(X, Y)$ will not be first countable so that questions of compactness, net convergence, and sequential convergence are complicated. The following simple example illustrates the different topologies on $\mathscr{L}(\ell_2)$.

Example Consider the bounded operators on ℓ_2.

(i) Let T_n be defined by

$$T_n(\xi_1, \xi_2, \ldots) = \left(\frac{1}{n}\xi_1, \frac{1}{n}\xi_2, \ldots\right)$$

Then $T_n \to 0$ uniformly.

(ii) Let S_n be defined by

$$S_n(\xi_1, \xi_2, \ldots) = (\underbrace{0, 0, \ldots, 0}_{n \text{ places}}, \xi_{n+1}, \xi_{n+2}, \ldots)$$

Then $S_n \to 0$ strongly but not uniformly.

(iii) Let W_n be defined by

$$W_n(\xi_1, \xi_2, \ldots) = (\underbrace{0, 0, \ldots, 0}_{n \text{ places}}, \xi_1, \xi_2, \ldots)$$

Then $W_n \to 0$ in the weak operator topology but not in the strong or uniform topologies.

The following result in the Hilbert space case is sometimes useful and provides a nice application of the uniform boundedness theorem.

Theorem VI.1 Let $\mathscr{L}(\mathscr{H})$ denote the bounded operators on a Hilbert space $\mathscr{H}$. Let T_n be a *sequence* of bounded operators and suppose that $(T_n x, y)$ converges as $n \to \infty$ for each $x, y \in \mathscr{H}$. Then there exists $T \in \mathscr{L}(\mathscr{H})$ such that $T_n \xrightarrow{w} T$.

Proof We begin by showing that for each x, $\sup_n \|T_n x\| < \infty$. Since for any $x \in \mathscr{H}$, $(x, T_n y)$ converges we have

$$\sup_n |(T_n x, y)| < \infty$$

For each n, $T_n x \in \mathscr{L}(\mathscr{H}, \mathbb{C})$, and since $\sup_n |(T_n x)(y)|_{\mathbb{C}} < \infty$, the uniform boundedness theorem implies that the operator norms of the $T_n x$ in $\mathscr{L}(\mathscr{H}, \mathbb{C})$ are uniformly bounded. But the norm of $T_n x$ as an operator in $\mathscr{L}(\mathscr{H}, \mathbb{C})$ is the same as its norm in $\mathscr{H}$; thus $\|T_n x\|_{\mathscr{H}}$ is uniformly bounded.

Now, we use the uniform boundedness theorem again. Since

$$\sup_n \|T_n x\|_{\mathscr{H}} < \infty,$$

we conclude

$$\sup_n \|T_n\|_{\mathscr{L}(\mathscr{H})} < \infty$$

Define $B(x, y) = \lim_n (T_n x, y)$. Then it is easily verified that $B(x, y)$ is sesquilinear and

$$|B(x, y)| \leq \overline{\lim_n} |(T_n x, y)| \leq \|x\| \|y\| (\sup_n \|T_n\|)$$

Thus $B(x, y)$ is a bounded sesquilinear form on $\mathscr{H}$ and so, by the corollary to the Riesz lemma, there is a bounded operator $T \in \mathscr{L}(\mathscr{H})$ such that $B(x, y) = (Tx, y)$. Clearly $T_n \xrightarrow{w} T$. ∎

If a *sequence* of operators T_n on a Hilbert space has the property that $T_n x$ converges for each $x \in \mathscr{H}$, then there exists $T \in \mathscr{L}(\mathscr{H})$ such that $T_n \xrightarrow{s} T$. The reader is asked to prove this theorem and various generalizations in Problem 3.

Let $T \in \mathscr{L}(X, Y)$. The set of vectors $x \in X$ so that $Tx = 0$ is called the **kernel** of T, written Ker T. The set of vectors $y \in Y$ so that $y = Tx$ for some $x \in X$ is called the **range** of T, written Ran T. Notice that both Ker T and Ran T are subspaces. Ker T is necessarily closed, but Ran T may not be closed (Problem 7).

VI.2 Adjoints

In this section we define adjoints of bounded operators on Banach and Hilbert spaces. The reader should be cautioned at the outset that the Hilbert space adjoint of an operator $T \in \mathscr{L}(\mathscr{H})$ is not equal to the Banach space adjoint although it is closely related to it.

Definition Let X and Y be Banach spaces, T a bounded linear operator from X to Y. The Banach space **adjoint** of T, denoted by T', is the bounded linear operator from Y^* to X^* defined by

$$(T'\ell)(x) = \ell(Tx)$$

for all $\ell \in Y^*$, $x \in X$.

Example Let $X = \ell_1 = Y$ and let T be the right shift operator

$$T(\xi_1, \xi_2, \ldots) = (0, \xi_1, \xi_2, \ldots)$$

Then $T' : \ell_\infty \to \ell_\infty$ is the operator

$$T'(\xi_1, \xi_2, \ldots) = (\xi_2, \xi_3, \ldots)$$

In this example, $\|T\| = 1 = \|T'\|$. In fact the norms of T and T' are always equal:

Theorem VI.2 Let X and Y be Banach spaces. The map $T \to T'$ is an isometric isomorphism of $\mathscr{L}(X, Y)$ *into* $\mathscr{L}(Y^*, X^*)$.

Proof The map $T \to T'$ is linear. The fact that T' is bounded and that the map is an isometry follows from the computation

$$\begin{aligned}
\|T\|_{\mathscr{L}(X,Y)} &= \sup_{\|x\| \le 1} \|Tx\|_Y \\
&= \sup_{\|x\| \le 1} \left(\sup_{\|\ell\| \le 1} |\ell(Tx)| \right) \qquad \ell \in Y^* \\
&= \sup_{\|\ell\| \le 1} \left(\sup_{\|x\| \le 1} |(T'\ell)(x)| \right) \\
&= \sup_{\|\ell\| \le 1} \|T'\ell\| \\
&= \|T'\|_{\mathscr{L}(Y^*, X^*)}
\end{aligned}$$

The second equality uses a corollary of the Hahn–Banach theorem. ∎

We are mostly interested in the case where T is a bounded linear transformation of a Hilbert space $\mathscr{H}$ to itself. The Banach space adjoint of T is then a mapping of $\mathscr{H}^*$ to $\mathscr{H}^*$. Let $C: \mathscr{H} \to \mathscr{H}^*$ be the map which assigns to each $y \in \mathscr{H}$, the bounded linear functional $(y, \cdot)$ in $\mathscr{H}^*$. C is a *conjugate* linear isometry which is surjective by the Riesz lemma. Now define a map T^*: $\mathscr{H} \to \mathscr{H}$ by

$$T^* = C^{-1}T'C$$

Then T^* satisfies

$$(x, Ty) = (Cx)(Ty) = (T'Cx)(y) = (C^{-1}T'Cx, y) = (T^*x, y)$$

T^* is called the **Hilbert space adjoint** of T, but usually we will just call it the adjoint and let the * distinguish it from T'. Notice that the map $T \to T^*$ is *conjugate* linear, that is, $\alpha T \to \bar{\alpha} T^*$. This is because C is conjugate linear. We summarize the properties of the map $T \to T^*$:

Theorem VI.3 (a) $T \to T^*$ is a conjugate linear isometric isomorphism of $\mathscr{L}(\mathscr{H})$ onto $\mathscr{L}(\mathscr{H})$.

(b) $(TS)^* = S^*T^*$.

(c) $(T^*)^* = T$.

(d) If T has a bounded inverse, T^{-1}, then T^* has a bounded inverse and $(T^*)^{-1} = (T^{-1})^*$.

(e) The map $T \to T^*$ is always continuous in the weak and uniform operator topologies but is only continuous in the strong operator topology if $\mathscr{H}$ is finite dimensional.

(f) $\|T^*T\| = \|T\|^2$.

Proof (a) follows from Theorem VI.2 and the fact that C is an isometry. (b) and (c) are easily checked. Since $T^{-1}T = I = TT^{-1}$ we have from (b)

$$T^*(T^{-1})^* = I^* = I = I^* = (T^{-1})^*T^*$$

which proves (d).

Continuity of $T \to T^*$ in the weak and uniform operator topologies is trivial. In the case $\mathscr{H} = \ell_2$, here is a counter example which shows that $T \to T^*$ is not continuous in the strong operator topology. The general infinite dimensional case is similar. Let W_n be right shift on ℓ_2 by n places. Then W_n converges weakly but not strongly to zero. However, $W_n^* = V_n$ converges strongly to zero. Thus $V_n \xrightarrow{s} 0$, but $V_n^* = W_n$ does not converge strongly to zero.

(f) Note that $\|T^*T\| \leq \|T\| \, \|T^*\| = \|T\|^2$ and

$$\|T^*T\| \geq \sup_{\|x\|=1} (x, T^*Tx) = \sup_{\|x\|=1} \|Tx\|^2 = \|T\|^2 \quad \blacksquare$$

Definition A bounded operator T on a Hilbert space is called **self-adjoint** if $T = T^*$.

Self-adjoint operators play a major role in functional analysis and mathematical physics and much of our time is devoted to studying them. Chapter VII is devoted to proving a structure theorem for bounded self-adjoint operators. In Chapter VIII we introduce unbounded self-adjoint operators and continue their study in Chapter X. We remind the reader that on $\mathbb{C}^n$, a linear transformation is self-adjoint if and only if its matrix in any orthonormal basis is invariant under the operation of reflection across the diagonal followed by complex conjugation.

An important class of operators on Hilbert spaces is that of the projections.

Definition If $P \in \mathscr{L}(\mathscr{H})$ and $P^2 = P$, then P is called a **projection**. If in addition $P = P^*$, then P is called an **orthogonal projection**.

Notice that the range of a projection is always a closed subspace on which P acts like the identity. If in addition P is orthogonal, then P acts like the zero operator on $(\text{Ran } P)^\perp$. If $x = y + z$, with $y \in \text{Ran } P$ and $z \in (\text{Ran } P)^\perp$, is the decomposition guaranteed by the projection theorem, then $Px = y$. P is called the orthogonal projection onto Ran P. Thus, the projection theorem sets up a

one to one correspondence between orthogonal projections and closed subspaces. Since orthogonal projections arise more frequently than non-orthogonal ones, we normally use the word projection to mean orthogonal projection.

VI.3 The spectrum

If T is a linear transformation on $\mathbb{C}^n$, then the eigenvalues of T are the complex numbers λ such that the determinant of $\lambda I - T$ is equal to zero. The set of such λ is called the spectrum of T. It can consist of at most n points since $\det(\lambda I - T)$ is a polynomial of degree n. If λ is not an eigenvalue, then $\lambda I - T$ has an inverse since $\det(\lambda I - T) \neq 0$.

The spectral theory of operators on infinite-dimensional spaces is more complicated, more interesting, and very important for an understanding of the operators themselves.

Definition Let $T \in \mathscr{L}(X)$. A complex number λ is said to be in the **resolvent set** $\rho(T)$ of T if $\lambda I - T$ is a bijection with a bounded inverse. $R_\lambda(T) = (\lambda I - T)^{-1}$ is called the **resolvent** of T at λ. If $\lambda \notin \rho(T)$, then λ is said to be in the **spectrum** $\sigma(T)$ of T.

We note that by the inverse mapping theorem, $\lambda I - T$ automatically has a bounded inverse if it is bijective. We distinguish two subsets of the spectrum.

Definition Let $T \in \mathscr{L}(X)$.

(a) An $x \neq 0$ which satisfies $Tx = \lambda x$ for some $\lambda \in \mathbb{C}$ is called an **eigenvector** of T; λ is called the corresponding **eigenvalue**. If λ is an eigenvalue, then $\lambda I - T$ is not injective so λ is in the spectrum of T. The set of all eigenvalues is called the **point spectrum** of T.

(b) If λ is not an eigenvalue and if $\operatorname{Ran}(\lambda I - T)$ is not dense, then λ is said to be in the **residual spectrum.**

At the end of this section we present an example which illustrates these kinds of spectra. The reason that we single out the residual spectrum is that it does not occur for a large class of operators, for example, for self-adjoint operators (see Theorem VI.8).

The spectral analysis of operators is very important for mathematical physics. For example, in quantum mechanics the Hamiltonian is an unbounded self-adjoint operator on a Hilbert space. The point spectrum of the Hamiltonian corresponds to the energy levels of bound states of the system. The rest of the spectrum plays an important role in the scattering theory of the system (see Chapter XII).

We will shortly prove that the resolvent set $\rho(T)$ is open and that $R_\lambda(T)$ is an analytic operator-valued function on $\rho(T)$. This fact allows one to use complex analysis to study $R_\lambda(T)$ and thus to obtain information about T. We begin with a brief aside about vector-valued analytic functions.

Let X be a Banach space and let D be a region in the complex plane, i.e., a connected open subset of $\mathbb{C}$. A function, $x(\cdot)$, defined on D with values in X, is said to be **strongly analytic** at $z_0 \in D$ if the limit of $(x(z_0 + h) - x(z_0))/h$ exists in X as h goes to zero in $\mathbb{C}$. Starting from this point one can develop a theory of vector-valued analytic functions which is almost exactly parallel to the usual theory; in particular, a strongly analytic function has a norm-convergent Taylor series. We do not repeat this development here; see the notes for references. We do want to discuss one important point. There is another natural way to define Banach-valued analytic functions. Namely: a function $x(\cdot)$ on D with values in X is said to be **weakly analytic** if $\ell(x(\cdot))$ is a complex valued analytic function on D for each $\ell \in X^*$. Although this second definition of analytic is a priori weaker than the first, the two definitions are equivalent, a fact we will prove in a moment. This is very important, since weak analyticity is often much easier to check.

Lemma Let X be a Banach space. Then a sequence $\{x_n\}$ is Cauchy if and only if $\{\ell(x_n)\}$ is Cauchy, uniformly for $\ell \in X^*$, $\|\ell\| \leq 1$.

Proof If $\{x_n\}$ is Cauchy, then $|\ell(x_n) - \ell(x_m)| \leq \|x_n - x_m\|$ for all ℓ with $\|\ell\| \leq 1$, so $\{\ell(x_n)\}$ is Cauchy uniformly. Conversely,

$$\|x_n - x_m\| = \sup_{\|\ell\| \leq 1} |\ell(x_n - x_m)|$$

Thus, if $\{\ell(x_n)\}$ is Cauchy, uniformly for $\|\ell\| \leq 1$, then $\{x_n\}$ is norm-Cauchy. ∎

Theorem VI.4 Every weakly analytic function is strongly analytic.

Proof Let $x(\cdot)$ be a weakly analytic function on D with values in X. Let

$z_0 \in D$ and suppose that Γ is a circle in D containing z_0 whose interior is contained in D. If $\ell \in X^*$ then $\ell(x(z))$ is analytic and

$$\ell\left(\frac{x(z_0+h)-x(z_0)}{h}\right) - \frac{d}{dz}\ell(x(z_0))$$
$$= \frac{1}{2\pi i}\oint_\Gamma \left[\frac{1}{h}\left(\frac{1}{z-(z_0+h)} - \frac{1}{z-z_0}\right) - \frac{1}{(z-z_0)^2}\right]\ell(x(z))\,dz$$

Since $\ell(x(z))$ is continuous on Γ and Γ is compact, $|\ell(x(z))| \le C_\ell$ for all $z \in \Gamma$. Regarding $x(z)$ as a family of mappings $x(z)\colon X^* \to \mathbb{C}$ we see that $x(z)$ is pointwise bounded at each ℓ so by the uniform boundedness theorem $\sup_{z\in\Gamma}\|x(z)\| \le C < \infty$. Thus

$$\left|\ell\left(\frac{x(z_0+h)-x(z_0)}{h}\right) - \frac{d}{dz}\ell(x(z_0))\right|$$
$$\le (2\pi)^{-1}\|\ell\|\left(\sup_{z\in\Gamma}\|x(z)\|\right)\oint_\Gamma \left|\frac{1}{(z-(z_0+h))(z-z_0)} - \frac{1}{(z-z_0)^2}\right| dz$$

This estimate shows that $[x(z_0+h)-x(z_0)]/h$ is uniformly Cauchy for $\|\ell\| \le 1$. By the lemma, $[x(z_0+h)-x(z_0)]/h$ converges in X, proving that $x(\cdot)$ is strongly analytic. ∎

We now prove the theorem we promised about the resolvent.

Theorem VI.5 Let X be a Banach space and suppose $T \in \mathscr{L}(X)$. Then $\rho(T)$ is an open subset of $\mathbb{C}$ and $R_\lambda(T)$ is an analytic $\mathscr{L}(X)$-valued function on each component (maximal connected subset) of D. For any two points λ, $\mu \in \rho(T)$, $R_\lambda(T)$ and $R_\mu(T)$ commute and

$$R_\lambda(T) - R_\mu(T) = (\mu-\lambda)R_\mu(T)R_\lambda(T) \tag{VI.1}$$

Proof We begin with the following formal computation, temporarily ignoring questions of convergence. Let $\lambda_0 \in \rho(T)$.

$$\frac{1}{\lambda - T} = \frac{1}{\lambda-\lambda_0+(\lambda_0-T)} = \left(\frac{1}{\lambda_0-T}\right)\frac{1}{1-\left(\frac{\lambda_0-\lambda}{\lambda_0-T}\right)}$$
$$= \left(\frac{1}{\lambda_0-T}\right)\left[1+\sum_{n=1}^{\infty}\left(\frac{\lambda_0-\lambda}{\lambda_0-T}\right)^n\right]$$

This suggests that we define

$$\tilde{R}_\lambda(T) = R_{\lambda_0}(T)\left\{I + \sum_{n=1}^{\infty}(\lambda_0-\lambda)^n[R_{\lambda_0}(T)]^n\right\}$$

Since

$$\|[R_{\lambda_0}(T)]^n\| \leq \|R_{\lambda_0}(T)\|^n$$

the series on the right converges in the uniform operator topology if

$$|\lambda - \lambda_0| < \|R_{\lambda_0}(T)\|^{-1}$$

For such λ, $\tilde{R}_\lambda(T)$ is well defined, and it is easily checked that

$$(\lambda I - T)\tilde{R}_\lambda(T) = I = \tilde{R}_\lambda(T)(\lambda I - T)$$

This proves that $\lambda \in \rho(T)$ if $|\lambda - \lambda_0| < \|R_{\lambda_0}(T)\|^{-1}$ and that $\tilde{R}_\lambda(T) = R_\lambda(T)$. Thus $\rho(T)$ is open. Since $R_\lambda(T)$ has a power series expansion, it is analytic.

The expression

$$R_\lambda(T) - R_\mu(T) = R_\lambda(T)(\mu I - T)R_\mu(T) - R_\lambda(T)(\lambda I - T)R_\mu(T)$$

proves (VI.1). Interchanging μ and λ shows that $R_\lambda(T)$ and $R_\mu(T)$ commute. ∎

Equation (VI.1) is called the **first resolvent formula**. A nice example of the use of complex analytic methods is given by the proof of the following corollary.

Corollary Let X be a Banach space, $T \in \mathcal{L}(X)$. Then the spectrum of T is not empty.

Proof Formally,

$$\frac{1}{\lambda - T} = \left(\frac{1}{\lambda}\right)\frac{1}{1 - T/\lambda} = \frac{1}{\lambda}\left(1 + \sum_{n=1}^{\infty}\left(\frac{T}{\lambda}\right)^n\right)$$

which suggests that for large values of $|\lambda|$,

$$R_\lambda(T) = \frac{1}{\lambda}\left\{I + \sum_{n=1}^{\infty}\left(\frac{T}{\lambda}\right)^n\right\} \tag{VI.2}$$

If $|\lambda| > \|T\|$, then the series on the right converges in norm and it is easily checked that for such λ, its limit is indeed the inverse of $(\lambda I - T)$. Thus, as $|\lambda| \to \infty$, $\|R_\lambda(T)\| \to 0$. If $\sigma(T)$ were empty, $R_\lambda(T)$ would be an entire bounded analytic function. By Liouville's theorem, $R_\lambda(T)$ would be zero which is a contradiction. Thus, $\sigma(T)$ is not empty. ∎

The series (VI.2) is called the **Neumann series** for $R_\lambda(T)$. The proof of the corollary shows that $\sigma(T)$ is contained in the closed disc of radius $\|T\|$. Actually, we can say more about $\sigma(T)$.

Definition Let $r(T) = \sup_{\lambda \in \sigma(T)} |\lambda|$

$r(T)$ is called the **spectral radius** of T.

Theorem VI.6 Let X be a Banach space, $T \in \mathscr{L}(X)$. Then $\lim_{n\to\infty} \|T^n\|^{1/n}$ exists and is equal to $r(T)$. If X is a Hilbert space and A is self-adjoint, then $r(A) = \|A\|$.

Proof The reader can check that $\lim_{n\to\infty} \|T^n\|^{1/n}$ exists by following the clever subadditivity argument outlined in Problem 11. The crux of the proof of the theorem is to establish that the radius of convergence of the Laurent series of $R_\lambda(T)$ about ∞ is just $r(T)^{-1}$. First notice that the radius of convergence cannot be smaller than $r(T)^{-1}$ since we have proven that $R_\lambda(T)$ is analytic on $\rho(T)$ and $\{\lambda \mid |\lambda| > r(T)\} \subset \rho(T)$. On the other hand, (VI.2) is just the Laurent series about ∞ and we have seen that where it converges absolutely, $R_\lambda(T)$ exists. Since a Laurent series converges absolutely inside the circle of convergence, we conclude that the radius of convergence cannot be larger than $r(T)^{-1}$. That $r(T) = \lim_{n\to\infty} \|T^n\|^{1/n}$ follows from the vector-valued version of Hadamard's theorem which says that the radius of convergence of (VI.2) is just the inverse of

$$\overline{\lim_n} \|T^n\|^{1/n} = \lim_{n\to\infty} \|T^n\|^{1/n}$$

Finally, if X is a Hilbert space and A is self-adjoint, then $\|A\|^2 = \|A^2\|$ by part (f) of Theorem VI.3. This implies that $\|A^{2^n}\| = \|A\|^{2^n}$ so

$$r(A) = \lim_{k\to\infty} \|A^k\|^{1/k} = \lim_{n\to\infty} \|A^{2^n}\|^{2^{-n}} = \|A\| \quad \blacksquare$$

The following theorem is sometimes useful in determining spectra.

Theorem VI.7 (Phillips) Let X be a Banach space, $T \in \mathscr{L}(X)$. Then $\sigma(T) = \sigma(T')$ and $R_\lambda(T') = R_\lambda(T)'$. If $\mathscr{H}$ is a Hilbert space, then $\sigma(T^*) = \{\lambda \mid \bar{\lambda} \in \sigma(T)\}$ and $R_\lambda(T^*) = R_\lambda(T)^*$.

We note that the Hilbert space case follows from (d) of Theorem VI.3.

We now work out in some detail an example which illustrates the various kinds of spectra.

Example Let T be the operator on ℓ_1 which acts by

$$T(\xi_1, \xi_2, \ldots) = (\xi_2, \xi_3, \ldots)$$

The adjoint of T, T', acts on ℓ_∞ by

$$T'(\xi_1, \xi_2, \ldots) = (0, \xi_1, \xi_2, \ldots)$$

We first observe that $\|T\| = \|T'\| = 1$, so that all λ with $|\lambda| > 1$ are in $\rho(T)$ and $\rho(T')$. Suppose $|\lambda| < 1$. Then the vector $x_\lambda = (1, \lambda, \lambda^2, \ldots)$ is in ℓ_1 and satisfies $(\lambda I - T)x_\lambda = 0$. Thus all such λ are in the point spectrum of T. Since the spectrum is closed, $\sigma(T) = \{\lambda \mid |\lambda| \leq 1\}$. By Theorem VI.7 this set is also the spectrum of T'.

We want to show that T' has no point spectrum. Suppose that $\{\xi_n\}_{n=1}^\infty \in \ell_\infty$ and $(\lambda I - T')\{\xi_n\} = 0$. Then

$$\begin{aligned} \lambda\xi_0 &= 0 \\ \lambda\xi_1 - \xi_0 &= 0 \\ &\vdots \end{aligned}$$

These equations together imply that $\{\xi_n\}_{n=1}^\infty = 0$ so $\lambda I - T'$ is one to one and T' has no point spectrum. Next, suppose $|\lambda| < 1$. Then for all $L \in \ell_\infty$

$$[(\lambda I - T')L](x_\lambda) = L((\lambda I - T)x_\lambda) = 0.$$

where $x_\lambda \in \ell_1$ is the eigenvector with eigenvalue λ. By the Hahn–Banach theorem we know that there is a linear functional in ℓ_∞ which does not vanish on x_λ so the range of $\lambda I - T'$ is not dense. Thus $\{\lambda; |\lambda| < 1\}$ is in the residual spectrum of T'.

It remains to consider the boundary $|\lambda| = 1$. Suppose that $|\lambda| = 1$ and $(\lambda I - T)\{\xi_n\} = 0$ for some $\{\xi_n\}$ in ℓ_1. Then

$$\begin{aligned} \xi_1 &= \lambda\xi_0 \\ \xi_2 &= \lambda\xi_1 \\ &\vdots \end{aligned}$$

so $\{\xi_n\}_{n=1}^\infty = \xi_0(1, \lambda, \lambda^2, \ldots)$ which is not in ℓ_1. Thus λ is not point spectrum. If the range of $\lambda I - T$ were not dense there would be a nonzero $L \in \ell_\infty$ such that $L[(\lambda I - T)x] = 0$ for all $x \in \ell_1$. But then $[(\lambda I - T')L](x) = 0$ which would imply that λ is in the point spectrum of T' which we have proven cannot occur. Thus, $\{\lambda \mid |\lambda| = 1\}$ is neither in the point spectrum of T nor in the residual spectrum of T.

Finally, we prove that $\{\lambda \mid |\lambda| = 1\}$ is in the residual spectrum of T' by explicitly finding an open ball disjoint from $\mathrm{Ran}(\lambda - T')$. If $a = \{a_n\}$ and $b = \{b_n\}$ are in ℓ_∞ and obey $a = (\lambda I - T')b$, then

$$\begin{aligned} a_0 &= \lambda b_0 \\ &\vdots \\ a_n &= \lambda b_n - b_{n-1} \end{aligned}$$

so $b_n = (\bar{\lambda})^{n+1} \sum_{m=0}^{n} \lambda^m a_m$. Let $c = \{c_n\}$ with $c_n = \bar{\lambda}^n$ and suppose that $d \in \ell_\infty$ and $\|d - c\|_\infty \leq \frac{1}{2}$. Then

$$\mathrm{Re}\{\lambda^n d_n\} \geq \mathrm{Re}\{\lambda^n c_n\} - \|d - c\|_\infty \geq \tfrac{1}{2}$$

Thus, if $(\lambda - T')e = d$ for some $e \in \ell_\infty$, then since

$$e_n = (\bar{\lambda})^{n+1} \sum_{m=0}^{n} \lambda^m d_m$$

$|e_n| \geq n/2$ which is impossible. Therefore, $\mathrm{Ran}(\lambda - T')$ does not intersect the ball of radius $\frac{1}{2}$ about c so λ is in the residual spectrum.

Operator	Spectrum	Point spectrum	Residual spectrum
T	$\lvert\lambda\rvert \leq 1$	$\lvert\lambda\rvert < 1$	$\varnothing$
T'	$\lvert\lambda\rvert \leq 1$	$\varnothing$	$\lvert\lambda\rvert \leq 1$

As in the above example, one can prove in general

Proposition Let X be a Banach space and $T \in \mathscr{L}(X)$. Then,

(a) If λ is in the residual spectrum of T, then λ is in the point spectrum of T'.
(b) If λ is in the point spectrum of T, then λ is in either the point or the residual spectrum of T'.

Finally, we note:

Theorem VI.8 Let T be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Then,

(a) T has no residual spectrum.
(b) $\sigma(T)$ is a subset of $\mathbb{R}$.
(c) Eigenvectors corresponding to distinct eigenvalues of T are orthogonal.

Proof If λ and μ are real, we compute

$$\|[T - (\lambda + i\mu)]x\|^2 = \|(T - \lambda)x\|^2 + \mu^2\|x\|^2$$

Thus $\|[T - (\lambda + i\mu)]x\|^2 \geq \mu^2\|x\|^2$, so if $\mu \neq 0$, then $T - (\lambda + i\mu)$ is one to one and has a bounded inverse on its range, which is closed. If $\mathrm{Ran}(T - (\lambda + i\mu)) \neq \mathscr{H}$, then, by the above proposition, $\lambda - i\mu$ would be in the point spectrum of T, which is impossible by the inequality. Thus if $\mu \neq 0$, $\lambda + i\mu$ is in $\rho(T)$. This proves (b). If a real λ were in the residual spectrum of T, then $\bar{\lambda} = \lambda$ would be in the point spectrum of $T^* = T$, which is impossible since the point and residual spectrum are disjoint by definition. This proves (a). The easy proof of (c) is left as an exercise (Problem 8). ∎

VI.4 Positive operators and the polar decomposition

We want to prove the existence of a special decomposition for operators on a *Hilbert space* which is analogous to the decomposition $z = |z|e^{i\arg z}$ for complex numbers. First we must describe a suitable analogue of the positive numbers.

Definition Let $\mathscr{H}$ be a Hilbert space. An operator $B \in \mathscr{L}(\mathscr{H})$ is called **positive** if $(Bx, x) \geq 0$ for all $x \in \mathscr{H}$. We write $B \geq 0$ if B is positive and $B \leq A$ if $A - B \geq 0$.

Every (bounded) positive operator on a *complex* Hilbert space is self-adjoint. To see this, notice that $(x, Ax) = \overline{(x, Ax)} = (Ax, x)$ if (Ax, x) takes only real values. By the polarization identity (Chapter II, Problem 4), $(Ax, y) = (x, Ay)$ if $(Ax, x) = (x, Ax)$ for all x. Thus, if A is positive, it is self-adjoint. This is false on real Hilbert spaces because it is not possible to recover (x, Ay) by knowing (x, Ax) for all x.

For any $A \in \mathscr{L}(\mathscr{H})$, notice that $A^*A \geq 0$ since $(A^*Ax, x) = \|Ax\|^2 \geq 0$. Just as $|z| = \sqrt{\bar{z}z}$ we would like to define $|A| = \sqrt{A^*A}$. To do this we must show that we can take square roots of positive operators. We begin with a lemma.

Lemma The power series for $\sqrt{1 - z}$ about zero converges absolutely for all complex numbers z satisfying $|z| \leq 1$.

Proof Let $\sqrt{1 - z} = 1 + c_1 z + c_2 z^2 + \cdots$ be the power series of $\sqrt{1 - z}$ about the origin. Since $\sqrt{1 - z}$ is analytic for $|z| < 1$, the series converges absolutely there. The derivatives of $\sqrt{1 - z}$ at the origin are all negative, so the c_i are negative if $i \geq 1$. Thus

$$\begin{aligned}
\sum_{n=0}^{N} |c_n| &= 2 - \sum_{n=0}^{N} c_n \\
&= 2 - \lim_{x \to 1-} \sum_{n=0}^{N} c_n x^n \\
&\leq 2 - \lim_{x \to 1-} \sqrt{1 - x} \\
&= 2
\end{aligned}$$

where $\lim_{x \to 1-}$ means the limit as x approaches one from below. Since this is true for all N, $\sum_{n=0}^{\infty} |c_n| \leq 2$, which implies that the series converges absolutely for $|z| = 1$. ∎

Theorem VI.9 (square root lemma) Let $A \in \mathscr{L}(\mathscr{H})$ and $A \geq 0$. Then there is a unique $B \in \mathscr{L}(\mathscr{H})$ with $B \geq 0$ and $B^2 = A$. Furthermore, B commutes with every bounded operator which commutes with A.

Proof It is sufficient to consider the case where $\|A\| \leq 1$. Since

$$\|I - A\| = \sup_{\|\varphi\| = 1} |((I - A)\varphi, \varphi)| \leq 1$$

the above lemma implies that the series $1 + c_1(I - A) + c_2(I - A)^2 + \cdots$ converges in norm to an operator B. Since the convergence is absolute we can square the series and rearrange terms which proves that $B^2 = A$. Furthermore, since $0 \leq I - A \leq I$ we have $0 \leq (\varphi, (I - A)^n\varphi) \leq 1$ for all $\varphi \in \mathscr{H}$ with $\|\varphi\| = 1$. Thus

$$(\varphi, B\varphi) = 1 + \sum_{n=1}^{\infty} c_n(\varphi, (I - A)^n\varphi)$$

$$\geq 1 + \sum_{n=1}^{\infty} c_n = 0$$

where we have used the fact that $c_n < 0$ and the estimate in the lemma. Thus, $B \geq 0$. Since the series for B converges absolutely, it commutes with any operator that commutes with A.

Suppose there is a B', with $B' \geq 0$ and $(B')^2 = A$. Then since

$$B'A = (B')^3 = AB'$$

B' commutes with A and thus with B. Therefore

$$(B - B')B(B - B') + (B - B')B'(B - B') = (B^2 - B'^2)(B - B') = 0 \qquad \text{(VI.3)}$$

Since both terms in (VI.3) are positive, they must both be zero, so their difference $(B - B')^3 = 0$. Since $B - B'$ is self-adjoint, $\|B - B'\|^4 = \|(B - B')^4\| = 0$, so $B - B' = 0$. ∎

We are now ready to define $|A|$.

Definition Let $A \in \mathscr{L}(\mathscr{H})$. Then $|A| = \sqrt{A^*A}$.

The reader should be wary of the emotional connotations of the symbol $|\cdot|$. While it is true that $|\lambda A| = |\lambda|\,|A|$ for $\lambda \in \mathbb{C}$, it is in general *false* that

$|AB| = |A|\,|B|$ or that $|A| = |A^*|$. Furthermore it is not true in general that $|A + B| \leq |A| + |B|$ (Problem 16). In fact, while it is known that $|\cdot|$ is norm continuous (see Problem 15), it is not known whether it is Lipschitz, that is, whether $\| |A| - |B| \| \leq c \|A - B\|$ for some constant c (however, see Problem 17).

The analogue of the complex numbers of modulus one is a little more complicated. At first one might expect that the unitary operators would be sufficient, but the following example shows that this is not the case.

Example Let A be the right shift operator on ℓ_2. Then $|A| = \sqrt{A^*A} = I$ so if we write $A = U|A|$ we must have $U = A$. However, A is not unitary since $(1, 0, 0, \ldots)$ is not in its range.

Definition An operator $U \in \mathscr{L}(\mathscr{H})$ is called an **isometry** if $\|Ux\| = \|x\|$ for all $x \in \mathscr{H}$. U is called a **partial isometry** if U is an isometry when restricted to the closed subspace $(\text{Ker } U)^\perp$.

Thus, if U is a partial isometry, $\mathscr{H}$ can be written as $\mathscr{H} = \text{Ker } U \oplus (\text{Ker } U)^\perp$ and $\mathscr{H} = \text{Ran } U \oplus (\text{Ran } U)^\perp$ and U is a unitary operator between $(\text{Ker } U)^\perp$, the **initial subspace** of U, and Ran U, the **final subspace** of U. It is not hard to see that U^* is a partial isometry from Ran U to $(\text{Ker } U)^\perp$ which acts as the inverse of the map U: $(\text{Ker } U)^\perp \to \text{Ran } U$.

Proposition Let U be a partial isometry. Then $P_i = U^*U$ and $P_f = UU^*$ are respectively the projections onto the initial and final subspaces of U. Conversely, if $U \in \mathscr{L}(\mathscr{H})$ with U^*U and UU^* projections, then U is a partial isometry.

The proof of the proposition is left to Problem 18. We are now ready to prove the analogue of the decomposition $z = |z|\, e^{i \arg z}$.

Theorem VI.10 (Polar decomposition) Let A be a bounded linear operator on a Hilbert space $\mathscr{H}$. Then there is a partial isometry U such that $A = U|A|$. U is uniquely determined by the condition that Ker U = Ker A. Moreover, Ran $U = \overline{\text{Ran } A}$.

Proof Define U: Ran $|A| \to$ Ran A by $U(|A|\,\psi) = A\psi$. Since

$$\| |A|\psi \|^2 = (\psi, |A|^2 \psi) = (\psi, A^*A\psi) = \|A\psi\|^2$$

U is well-defined, that is, if $|A|\psi = |A|\phi$ then $A\psi = A\phi$. U is isometric and so extends to an isometry of $\overline{\text{Ran}\,|A|}$ to $\overline{\text{Ran}\,A}$. Extend U to all of $\mathscr{H}$ by defining it to be zero on $(\text{Ran}\,|A|)^{\perp}$. Since $|A|$ is self-adjoint, $(\text{Ran}\,|A|)^{\perp} = \text{Ker}\,|A|$. Furthermore, $|A|\psi = 0$ if and only if $A\psi = 0$ so that $\text{Ker}\,|A| = \text{Ker}\,A$. Thus $\text{Ker}\,U = \text{Ker}\,A$. Uniqueness is left to the reader. ∎

In Problem 20 of Chapter VII, the reader will prove that U is a strong limit of polynomials in A and A^* so that U is in the "von Neumann algebra" generated by A.

VI.5 Compact operators †

Many problems in classical mathematical physics can be handled by reformulating them in terms of integral equations. A famous example is the Dirichlet problem discussed at the end of this section. Consider the simple operator K, defined in $C[0, 1]$ by

$$(K\varphi)(x) = \int_0^1 K(x, y)\varphi(y)\, dy \tag{VI.4}$$

where the function $K(x, y)$ is continuous on the square $0 \le x, y \le 1$. $K(x, y)$ is called the **kernel** of the **integral operator** K. Since

$$|(K\varphi)(x)| \le \left(\sup_{0\le x,\, y\le 1} |K(x, y)|\right)\left(\sup_{0\le y\le 1} |\varphi(y)|\right)$$

we see that

$$\|K\varphi\|_\infty \le \left(\sup_{0\le x,\, y<1} |K(x, y)|\right)\|\varphi\|_\infty$$

so K is a bounded operator on $C[0, 1]$. K has another property which is very important. Let B_M denote the functions φ in $C[0, 1]$ such that $\|\varphi\|_\infty \le M$. Since $K(x, y)$ is continuous on the square $0 \le x, y \le 1$ and since the square is compact, $K(x, y)$ is uniformly continuous. Thus, given an $\varepsilon > 0$, we can find $\delta > 0$ such that $|x - x'| < \delta$ implies $|K(x, y) - K(x', y)| < \varepsilon$ for all $y \in [0, 1]$. Thus, if $\varphi \in B_M$

$$\begin{aligned}|(K\varphi)(x) - (K\varphi)(x')| &\le \left(\sup_{y\in[0,\,1]} |K(x, y) - K(x', y)|\right)\|\varphi\|_\infty \\ &\le \varepsilon M\end{aligned}$$

† A supplement to this section begins on p. 368.

Therefore the functions $K[B_M]$ are equicontinuous. Since they are also uniformly bounded by $\|K\|M$, we can use the Ascoli theorem (Theorem I.28) to conclude that for every sequence $\varphi_n \in B_M$, the sequence $K\varphi_n$ has a convergent subsequence (the limit may not be in $K[B_M]$). Another way of saying this is that the set $K[B_M]$ is **precompact**; that is, its closure is compact in $C[0, 1]$. It is clear that the choice of M was not important so what we have shown is that K takes bounded sets into precompact sets. It is this property which makes the so called "Fredholm alternative" hold for nice integral equations like (VI.4). This section is devoted to studying such operators.

Definition Let X and Y be Banach spaces. An operator $T \in \mathscr{L}(X, Y)$ is called **compact** (or completely continuous) if T takes bounded sets in X into precompact sets in Y. Equivalently, T is compact if and only if for every bounded sequence $\{x_n\} \subset X$, $\{Tx_n\}$ has a subsequence convergent in Y.

The integral operator (VI.4) is one example of a compact operator. Another class of examples is:

Example (finite rank operators) Suppose that the range of T is finite dimensional. That is, every vector in the range of T can be written $Tx = \sum_{i=1}^{N} \alpha_i y_i$, for some fixed family $\{y_i\}_{i=1}^{N}$ in Y. If x_n is any bounded sequence in X, the corresponding α_i^n are bounded since T is bounded. The usual subsequence trick allows one to extract a convergent subsequence from $\{Tx_n\}$ which proves that T is compact.

An important property of compact operators is given by (compare Problem 34):

Theorem VI.11 A compact operator maps weakly convergent *sequences* into norm convergent sequences.

Proof Suppose $x_n \overset{w}{\to} x$. By the uniform boundedness theorem, the $\|x_n\|$ are bounded. Let $y_n = Tx_n$. Then $\ell(y_n) - \ell(y) = (T'\ell)(x_n - x)$ for any $\ell \in Y^*$. Thus, y_n converges weakly to $y = Tx$ in Y. Suppose that y_n does not converge to y in norm. Then, there is an $\varepsilon > 0$ and a subsequence $\{y_{n_k}\}$ of $\{y_n\}$ so that $\|y_{n_k} - y\| \geq \varepsilon$. Since the sequence $\{x_{n_k}\}$ is bounded and T is compact $\{y_{n_k}\}$ has a subsequence which converges to a $\tilde{y} \neq y$. This subsequence must then also converge weakly to $\tilde{y}$, but this is impossible since y_n converges weakly to y. Thus y_n converges to y in norm. ∎

We note that if X is reflexive then the converse of Theorem VI.11 holds (Problem 20). The following theorem is important since one can use it to prove that an operator is compact by exhibiting it as a norm limit of compact operators or as an adjoint of a compact operator.

Theorem VI.12 Let X and Y be Banach spaces, $T \in \mathscr{L}(X, Y)$.

(a) If $\{T_n\}$ are compact and $T_n \to T$ in the norm topology, then T is compact.

(b) T is compact if and only if T' is compact.

(c) If $S \in \mathscr{L}(Y, Z)$ with Z a Banach space and if T *or* S is compact, then ST is compact.

Proof (a) Let $\{x_m\}$ be a sequence in the unit ball of X. Since T_n is compact for each n, we can use the diagonalization trick of I.5 to find a subsequence of $\{x_m\}$, call it $\{x_{m_k}\}$, so that $T_n x_{m_k} \to y_n$ for each n as $k \to \infty$. Since $\|x_{m_k}\| \leq 1$ and $\|T_n - T\| \to 0$, an $\varepsilon/3$-argument shows that the sequence $\{y_n\}$ is Cauchy, so $y_n \to y$. It is not difficult to show using an $\varepsilon/3$ argument that $Tx_{m_k} \to y$. Thus T is compact.

(b) See the Notes and Problem 36.

(c) The proof is elementary (Problem 37). ∎

We are mostly interested in the case where T is a compact operator from a separable Hilbert space to itself, so we will not pursue the general case any further (however, see the discussion in the Notes). We denote the Banach space of compact operators on a separable Hilbert space by $\mathrm{Com}(\mathscr{H})$. By the first example and Theorem VI.12 the norm limit of a sequence of finite rank operators is compact. The converse is also true in the Hilbert space case.

Theorem VI.13 Let $\mathscr{H}$ be a separable Hilbert space. Then every compact operator on $\mathscr{H}$ is the norm limit of a sequence of operators of finite rank.

Proof Let $\{\varphi_j\}_{j=1}^{\infty}$ be an orthonormal set in $\mathscr{H}$. Define

$$\lambda_n = \sup_{\substack{\psi \in [\varphi_1, \ldots, \varphi_n]^{\perp} \\ \|\psi\| = 1}} \|T\psi\|$$

Clearly, $\{\lambda_n\}$ is monotone decreasing so it converges to a limit $\lambda \geq 0$. We first show that $\lambda = 0$. Choose a sequence $\psi_n \in [\varphi_1, \ldots, \varphi_n]^{\perp}$, $\|\psi_n\| = 1$, with

$\|T\psi_n\| \geq \lambda/2$. Since $\psi_n \overset{w}{\to} 0$, $T\psi_n \to 0$ by Theorem VI.11. Thus, $\lambda = 0$. As a result

$$\sum_{j=1}^{n} (\varphi_j, \cdot)T\varphi_j \to T$$

in norm since λ_n is just the norm of the difference. ∎

We have discussed a wide variety of properties of compact operators but we have not yet described any property which explains our special interest in them. The basic principle which makes compact operators important is the Fredholm alternative: If A is compact, then either $A\psi = \psi$ has a solution or $(I - A)^{-1}$ exists. This is not a property shared by all bounded linear transformations. For example, if A is the operator $(A\varphi)(x) = x\varphi(x)$ on $L^2[0, 2]$, then $A\varphi = \varphi$ has no solutions but $(I - A)^{-1}$ does not exist (as a bounded operator). In terms of "solving equations" the Fredholm alternative is especially nice: It tells us that if for any φ there is at most one ψ with $\psi = \varphi + A\psi$, then there is always exactly one. That is, compactness and uniqueness together imply existence; for an example, see the discussion of the Dirichlet problem at the end of the section.

As one might expect, since the Fredholm alternative holds for finite-dimensional matrices, it is possible to prove the Fredholm alternative for compact operators (in the Hilbert space case) by using the fact that any compact operator A can be written as $A = F + R$ where F has finite rank and R has small norm. Compactness combines very nicely with analyticity so we first prove an elegant result which is of great use in itself (see Sections XI.6, XI.7, XIII.4, and XIII.5).

Theorem VI.14 (analytic Fredholm theorem) Let D be an open connected subset of $\mathbb{C}$. Let $f\colon D \to \mathscr{L}(\mathscr{H})$ be an analytic operator-valued function such that $f(z)$ is compact for each $z \in D$. Then, either

(a) $(I - f(z))^{-1}$ exists for no $z \in D$.

or

(b) $(I - f(z))^{-1}$ exists for all $z \in D\backslash S$ where S is a discrete subset of D (i.e. a set which has no limit points in D). In this case, $(I - f(z))^{-1}$ is meromorphic in D, analytic in $D\backslash S$, the residues at the poles are finite rank operators, and if $z \in S$ then $f(z)\psi = \psi$ has a nonzero solution in $\mathscr{H}$.

Proof We will prove that near any z_0 either (a) or (b) holds. A simple connectedness argument allows one to convert this into a statement about all of D

(Problem 21). Given $z_0 \in D$, choose an r so that $|z - z_0| < r$ implies $\|f(z) - f(z_0)\| < \frac{1}{2}$ and pick F, an operator with finite rank so that

$$\|f(z_0) - F\| < \tfrac{1}{2}$$

Then, for $z \in D_r$, the disc of radius r about z_0, $\|f(z) - F\| < 1$. By expanding in a geometric series we see that $(I - f(z) + F)^{-1}$ exists and is analytic.

Since F has finite rank, there are independent vectors $\psi_1, \ldots, \psi_N$ so that $F(\varphi) = \sum_{i=1}^{N} \alpha_i(\varphi)\psi_i$. The $\alpha_i(\cdot)$ are bounded linear functionals on $\mathscr{H}$ so by the Riesz lemma there are vectors $\phi_1, \ldots, \phi_N$ so that $F(\varphi) = \sum_{n=1}^{N} (\phi_i, \varphi)\psi_i$ for all $\varphi \in \mathscr{H}$. Let $\phi_n(z) = ((I - f(z) + F)^{-1})^* \phi_n$ and

$$g(z) = F(I - f(z) + F)^{-1} = \sum_{n=1}^{N} (\phi_n(z), \cdot)\psi_n$$

By writing

$$(I - f(z)) = (I - g(z))(I - f(z) + F)$$

we see that $I - f(z)$ is invertible for $z \in D_r$ if and only if $I - g(z)$ is invertible and that $\psi = f(z)\psi$ has a nonzero solution if and only if $\varphi = g(z)\varphi$ has a solution.

If $g(z)\varphi = \varphi$, then $\varphi = \sum_{n=1}^{N} \beta_n \psi_n$ and the β_n satisfy

$$\beta_n = \sum_{m=1}^{N} (\phi_n(z), \psi_m)\beta_m \tag{VI.5a}$$

Conversely, if (VI.5a) has a solution $\langle \beta_1, \ldots, \beta_N \rangle$, then $\varphi = \sum_{n=1}^{N} \beta_n \psi_n$ is a solution of $g(z)\varphi = \varphi$. Thus $g(z)\varphi = \varphi$ has a solution if and only if the determinant

$$d(z) = \det\{\delta_{nm} - (\phi_n(z), \psi_m)\} = 0$$

Since $(\phi_n(z), \psi_m)$ is analytic in D_r so is $d(z)$ which means that either $S_r = \{z \mid z \in D_r, d(z) = 0\}$ is a discrete set in D_r or $S_r = D_r$. Now, suppose $d(z) \neq 0$. Then, given ψ, we can solve $(I - g(z))\varphi = \psi$ by setting $\varphi = \psi + \sum_{n=1}^{N} \beta_n \psi_n$ if we can find β_n satisfying

$$\beta_n = (\phi_n(z), \psi) + \sum_{m=1}^{N} (\phi_n(z), \psi_m)\beta_m \tag{VI.5b}$$

But, since $d(z) \neq 0$, this equation has a solution. Thus $(I - g(z))^{-1}$ exists if and only if $z \notin S_r$.

The meromorphic nature of $(I - f(z))^{-1}$ and the finite rank residues follow from the fact that there is an explicit formula for the β_n in (VI.5b) in terms of cofactor matrices. ∎

This theorem has four important consequences:

Corollary (the Fredholm alternative) If A is a compact operator on $\mathscr{H}$, then either $(I - A)^{-1}$ exists or $A\psi = \psi$ has a solution.

Proof Take $f(z) = zA$ and apply the last theorem at $z = 1$. ∎

Theorem VI.15 (Riesz–Schauder theorem) Let A be a compact operator on $\mathscr{H}$, then $\sigma(A)$ is a discrete set having no limit points except perhaps $\lambda = 0$. Further, any nonzero $\lambda \in \sigma(A)$ is an eigenvalue of finite multiplicity (i.e. the corresponding space of eigenvectors is finite dimensional).

Proof Let $f(z) = zA$. Then $f(z)$ is an analytic compact operator-valued function on the entire plane. Thus $\{z \mid zA\psi = \psi$ has a solution $\psi \neq 0\}$ is a discrete set (it is not the entire plane since it does not contain $z = 0$) and if $1/\lambda$ is not in this discrete set then

$$(\lambda - A)^{-1} = \frac{1}{\lambda}\left(I - \frac{1}{\lambda}A\right)^{-1}$$

exists. The fact that the nonzero eigenvalues have finite multiplicity follows immediately from the compactness of A. ∎

Theorem VI.16 (the Hilbert–Schmidt theorem) Let A be a self-adjoint compact operator on $\mathscr{H}$. Then, there is a complete orthonormal basis, $\{\phi_n\}$, for $\mathscr{H}$ so that $A\phi_n = \lambda_n \phi_n$ and $\lambda_n \to 0$ as $n \to \infty$.

Proof For each eigenvalue of A choose an orthonormal basis for the set of eigenvectors corresponding to the eigenvalue. The collection of all these vectors, $\{\phi_n\}$, is an orthonormal set since eigenvectors corresponding to distinct eigenvalues are orthogonal. Let $\mathscr{M}$ be the closure of the span of $\{\phi_n\}$. Since A is self-adjoint and $A\colon \mathscr{M} \to \mathscr{M}$, $A\colon \mathscr{M}^\perp \to \mathscr{M}^\perp$. Let $\tilde{A}$ be the restriction of A to $\mathscr{M}^\perp$. Then $\tilde{A}$ is self-adjoint and compact since A is. By the Riesz–Schauder theorem, if any $\lambda \neq 0$ is in $\sigma(\tilde{A})$, it is an eigenvalue of $\tilde{A}$ and thus of A. Therefore the spectral radius of $\tilde{A}$ is zero since the eigenvectors of A are in $\mathscr{M}$. Because $\tilde{A}$ is self-adjoint, it is the zero operator on $\mathscr{M}^\perp$ by Theorem VI.6. Thus, $\mathscr{M}^\perp = \{0\}$ since if $\varphi \in \mathscr{M}^\perp$, then $A\varphi = 0$ which implies that $\varphi \in \mathscr{M}$. Therefore, $\mathscr{M} = \mathscr{H}$.

The fact that $\lambda_n \to 0$ is a consequence of the first part of the Riesz–Schauder theorem which says that each nonzero eigenvalue has finite multiplicity and the only possible limit point of the λ_n is zero. ∎

Theorem VI.17 (canonical form for compact operators) Let A be a compact operator on $\mathscr{H}$. Then there exist (not necessarily complete)

orthonormal sets $\{\psi_n\}_{n=1}^N$ and $\{\phi_n\}_{n=1}^N$ and positive real numbers $\{\lambda_n\}_{n=1}^N$ with $\lambda_n \to 0$ so that

$$A = \sum_{n=1}^{N} \lambda_n(\psi_n, \cdot)\phi_n \tag{VI.6}$$

The sum in (VI.6), which may be finite or infinite, converges in norm. The numbers, $\{\lambda_n\}$, are called the **singular values** of A.

Proof Since A is compact, so is A^*A (Theorem VI.12). Thus A^*A is compact and self-adjoint. By the Hilbert–Schmidt theorem, there is an orthonormal set $\{\psi_n\}_{n=1}^N$ so that $A^*A\psi_n = \mu_n\psi_n$ with $\mu_n \neq 0$ and so that A^*A is the zero operator on the subspace orthogonal to $\{\psi_n\}_{n=1}^N$. Since A^*A is positive, each $\mu_n > 0$. Let λ_n be the positive square root of μ_n and set $\phi_n = A\psi_n/\lambda_n$. A short calculation shows that the ϕ_n are orthonormal and that

$$A\psi = \sum_{n=1}^{N} \lambda_n(\psi_n, \psi)\phi_n \quad \blacksquare$$

The proof shows that the singular values of A are precisely the eigenvalues of $|A|$.

We conclude with a classical example.

Example (Dirichlet problem) The main impetus for the study of compact operators arose from the use of integral equations in attempting to solve the classical boundary value problems of mathematical physics. We briefly describe this method. Let D be an open bounded region in $\mathbb{R}^3$ with a smooth boundary surface ∂D. The Dirichlet problem for Laplace's equation is: given a continuous function f on ∂D, find a function u, twice differentiable in D and continuous on $\bar{D}$, which satisfies

$$\begin{aligned} \Delta u(x) &= 0 \qquad x \in D \\ u(x) &= f(x) \qquad x \in \partial D \end{aligned}$$

Let $K(x, y) = (x - y, n_y)/2\pi|x - y|^3$ where n_y is the outer normal to ∂D at the point $y \in \partial D$. Then, as a function of x, $K(x, y)$ satisfies $\Delta_x K(x, y) = 0$ in the interior which suggests that we try to write u as a superposition

$$u(x) = \int_{\partial D} K(x, y)\varphi(y)\, dS(y) \tag{VI.6a}$$

where $\varphi(y)$ is some continuous function on ∂D and dS is the usual surface measure. Indeed, for $x \in D$, the integral makes perfectly good sense and

$\Delta u(x) = 0$ in D. Furthermore, if x_0 is any point in ∂D and $x \to x_0$ from *inside* D, it can be proven that

$$u(x) \to -\varphi(x_0) + \int_{\partial D} K(x_0, y)\varphi(y)\, dS(y) \tag{VI.6b}$$

If $x \to x_0$ from outside D, the minus is replaced by a plus. Also,

$$\int_{\partial D} K(x_0, y)\varphi(y)\, dS(y)$$

exists and is a continuous function on ∂D if φ is a continuous function on ∂D. The proof depends on the fact that the boundary of D is smooth which implies that for $x, y \in \partial D$, $(x - y, n_y) \approx c|x - y|^2$ as $x \to y$.

Since we wish $u(x) = f(x)$ on ∂D, the whole question reduces to whether we can find φ so that

$$f(x) = -\varphi(x) + \int_{\partial D} K(x, y)\varphi(y)\, dS(y), \qquad x \in \partial D$$

Let T: $C(\partial D) \to C(\partial D)$ be defined by

$$T\varphi = \int_{\partial D} K(x, y)\varphi(y)\, dS(y)$$

Not only is T bounded but (as we will shortly see) T is also compact. Thus, by the Fredholm alternative, either $\lambda = 1$ is in the point spectrum of T in which case there is a $\psi \in C(\partial D)$ such that $(I - T)\psi = 0$, or $-f = (I - T)\varphi$ has a unique solution for each $f \in C(\partial D)$. If u is defined by (VI.6a) with ψ replacing φ, then $u \equiv 0$ in D by the maximum principle. Further, $\partial u/\partial n$ is continuous across ∂D and therefore equals zero on ∂D. By an integration by parts this implies that $u \equiv 0$ outside ∂D. Therefore, by (VI.6b), $2\psi(x) \equiv 0$ on ∂D, so the first alternative does not hold.

The idea of the compactness proof is the following. Let

$$K_\delta(x, z) = \frac{(x - z, n_z)}{|x - z|^3 + \delta}$$

If $\delta > 0$, the kernel K_δ is continuous, so, by the discussion at the beginning of this section, the corresponding integral operators T_δ, are compact. To prove that T is compact, we need only show that $\|T - T_\delta\| \to 0$ as $\delta \to 0$. By the estimate

$$|(T_\delta f)(x) - (Tf)(x)| \le \|f\|_\infty \int_{\partial D} |K(x, z) - K_\delta(x, z)|\, dS(z)$$

we must only show that the integral converges to zero uniformly in x as $\delta \to 0$. To prove this, divide the integration region into the set where $|x-z| \geq \varepsilon$ and its complement. For fixed ε, the kernels converge uniformly on the first region. By using the fact that K is integrable, the contribution from the second region can be made arbitrarily small for ε sufficiently small.

VI.6 The trace class and Hilbert–Schmidt ideals

In the last section we saw that compact operators have many nice properties and are useful for applications. It is therefore important to have effective criteria for determining when a given operator is compact or, better yet, general statements about whole classes of operators. In this section we will prove that the integral operator

$$(Tf)(x) = \int_M K(x, y) f(y)\, d\mu(y)$$

on $L^2(M, d\mu)$ is compact if $K(\cdot, \cdot) \in L^2(M \times M, d\mu \otimes d\mu)$. First we will develop the trace, a tool which is of great interest in itself. Theorem VI.12 shows that $\mathrm{Com}(\mathscr{H})$, the compact operators on a separable Hilbert space $\mathscr{H}$, form a Banach space. At the conclusion of the section, we will compute the dual and double dual of $\mathrm{Com}(\mathscr{H})$. These calculations illustrate the difference between the weak Banach space topology on $\mathscr{L}(\mathscr{H})$ and the weak operator topology and give a foretaste of the structure of abstract von Neumann algebras which we will study later.

The trace is a generalization of the usual notion of the sum of the diagonal elements of a matrix, but because infinite sums are involved, not all operators will have a trace. The construction of the trace is analogous to the construction of the Lebesgue integral where one first defines $\int f\, d\mu$ for $f \geq 0$; it has values in $[0, \infty]$, including ∞. Then $\mathscr{L}^1$ is defined as those f so that $\int |f|\, d\mu < \infty$. $\mathscr{L}^1$ is a vector space and $f \mapsto \int f\, d\mu$ a linear functional. Similarly we first define the trace, $\mathrm{tr}(\cdot)$, on the positive operators; $A \to \mathrm{tr}\, A$ has values in $[0, \infty]$. We then define the **trace class**, $\mathscr{I}_1$, to be all $A \in \mathscr{L}(\mathscr{H})$ such that $\mathrm{tr}\, |A| < \infty$. We will then show that $\mathrm{tr}(\cdot)$ is a linear functional on $\mathscr{I}_1$ with the right properties.

Theorem VI.18 Let $\mathscr{H}$ be a separable Hilbert space, $\{\varphi_n\}_{n=1}^{\infty}$ an orthonormal basis. Then for any positive operator $A \in \mathscr{L}(\mathscr{H})$ we define $\mathrm{tr}\, A = \sum_{n=1}^{\infty} (\varphi_n, A\varphi_n)$. The number $\mathrm{tr}\, A$ is called the **trace of** A and is independent of the orthonormal basis chosen. The trace has the following properties:

(a) $\operatorname{tr}(A+B) = \operatorname{tr} A + \operatorname{tr} B$.
(b) $\operatorname{tr}(\lambda A) = \lambda \operatorname{tr} A$ for all $\lambda \geq 0$.
(c) $\operatorname{tr}(UAU^{-1}) = \operatorname{tr} A$ for any unitary operator U.
(d) If $0 \leq A \leq B$, then $\operatorname{tr} A \leq \operatorname{tr} B$.

Proof Given an orthonormal basis $\{\varphi_n\}_{n=1}^{\infty}$, define $\operatorname{tr}_{\varphi}(A) = \sum_{n=1}^{\infty} (\varphi_n, A\varphi_n)$. If $\{\psi_m\}_{m=1}^{\infty}$ is another orthonormal basis then

$$\begin{aligned}
\operatorname{tr}_{\varphi}(A) &= \sum_{n=1}^{\infty} (\varphi_n, A\varphi_n) = \sum_{n=1}^{\infty} \|A^{1/2}\varphi_n\|^2 \\
&= \sum_{n=1}^{\infty} \left(\sum_{m=1}^{\infty} |(\psi_m, A^{1/2}\varphi_n)|^2 \right) \\
&= \sum_{m=1}^{\infty} \left(\sum_{n=1}^{\infty} |(A^{1/2}\psi_m, \varphi_n)|^2 \right) \\
&= \sum_{m=1}^{\infty} \|A^{1/2}\psi_m\|^2 \\
&= \sum_{m=1}^{\infty} (\psi_m, A\psi_m) \\
&= \operatorname{tr}_{\psi}(A)
\end{aligned}$$

Since all the terms are positive, interchanging the sums is allowed.

Properties (a), (b), and (d) are obvious. To prove (c) we note that if $\{\varphi_n\}$ is an orthonormal basis, then so is $\{U\varphi_n\}$. Thus,

$$\operatorname{tr}(UAU^{-1}) = \operatorname{tr}_{(U\varphi)}(UAU^{-1}) = \operatorname{tr}_{\varphi}(A) = \operatorname{tr}(A). \quad \blacksquare$$

Definition An operator $A \in \mathscr{L}(\mathscr{H})$ is called **trace class** if and only if $\operatorname{tr}|A| < \infty$. The family of all trace class operators is denoted by $\mathscr{I}_1$.

The basic properties of $\mathscr{I}_1$ are given in the following:

Theorem VI.19 $\mathscr{I}_1$ is a $*$-ideal in $\mathscr{L}(\mathscr{H})$, that is,

(a) $\mathscr{I}_1$ is a vector space.
(b) If $A \in \mathscr{I}_1$ and $B \in \mathscr{L}(\mathscr{H})$, then $AB \in \mathscr{I}_1$ and $BA \in \mathscr{I}_1$.
(c) If $A \in \mathscr{I}_1$, then $A^* \in \mathscr{I}_1$.

Proof (a) Since $|\lambda A| = |\lambda|\,|A|$ for $\lambda \in \mathbb{C}$, $\mathscr{I}_1$ is closed under scalar multiplication. Now, suppose that A and B are in $\mathscr{I}_1$, we wish to prove that

$A + B \in \mathscr{I}_1$. Let U, V, and W be the partial isometries arising from the polar decompositions

$$A + B = U|A + B|$$
$$A = V|A|$$
$$B = W|B|$$

Then

$$\sum_{n=1}^{N} (\varphi_n, |A + B|\varphi_n) = \sum_{n=1}^{N} (\varphi_n, U^*(A + B)\varphi_n)$$
$$\leq \sum_{n=1}^{N} |(\varphi_n, U^*V|A|\varphi_n)| + \sum_{n=1}^{N} |(\varphi_n, U^*W|B|\varphi_n)|$$

However,

$$\sum_{n=1}^{N} |(\varphi_n, U^*V|A|\varphi_n)| \leq \sum_{n=1}^{N} \| \, |A|^{1/2}V^*U\varphi_n\| \, \| \, |A|^{1/2}\varphi_n\|$$
$$\leq \left(\sum_{n=1}^{N} \| \, |A|^{1/2}V^*U\varphi_n\|^2\right)^{1/2} \left(\sum_{n=1}^{N} \| \, |A|^{1/2}\varphi_n\|^2\right)^{1/2}$$

Thus, if we can show

$$\sum_{n=1}^{N} \| \, |A|^{1/2}V^*U\varphi_n\|^2 \leq \operatorname{tr} |A| \tag{VI.7}$$

we can conclude that

$$\sum_{n=1}^{N} (\varphi_n, |A + B|\varphi_n) \leq \operatorname{tr} |A| + \operatorname{tr} |B| < \infty$$

and thus $A + B \in \mathscr{I}_1$. To show (VI.7), we need only prove that

$$\operatorname{tr}(U^*V|A|V^*U) \leq \operatorname{tr}|A|$$

Picking an orthonormal basis, $\{\varphi_n\}$ with each φ_n in Ker U or (Ker U)$^\perp$ we see that $\operatorname{tr}(U^*(V|A|V^*)U) \leq \operatorname{tr}(V|A|V^*)$. Similarly, picking an orthonormal basis, $\{\psi_m\}$, with each ψ_m in Ker V^* or (Ker V^*)$^\perp$ we find $\operatorname{tr}(V|A|V^*) \leq \operatorname{tr} |A|$.

(b) By the lemma proven below, each $B \in \mathscr{L}(\mathscr{H})$ can be written as a linear combination of four unitary operators so by (a) we need only show that $A \in \mathscr{I}_1$ implies $UA \in \mathscr{I}_1$ and $AU \in \mathscr{I}_1$ if U is unitary. But $|UA| = |A|$ and $|AU| = U^{-1}|A|U$, so by part (c) of Theorem VI.18, AU and UA are in $\mathscr{I}_1$.

(c) Let $A = U|A|$ and $A^* = V|A^*|$ be the polar decompositions of A and A^*. Then $|A^*| = V^*|A|U^*$. If $A \in \mathscr{I}_1$, then $|A| \in \mathscr{I}_1$, so by part (b) $|A^*| \in \mathscr{I}_1$ and $A^* = V|A^*| \in \mathscr{I}_1$. ∎

To complete the proof of part (b) above we need the following lemma which we will use in other contexts later.

Lemma Every $B \in \mathscr{L}(\mathscr{H})$ can be written as a linear combination of four unitary operators.

Proof Since $B = \frac{1}{2}(B + B^*) - \frac{i}{2}[i(B - B^*)]$, B can be written as a linear combination of two self-adjoint operators. So, suppose A is self-adjoint and without loss of generality assume $\|A\| \leq 1$. Then $A \pm i\sqrt{I - A^2}$ are unitary and $A = \frac{1}{2}(A + i\sqrt{I - A^2}) + \frac{1}{2}(A - i\sqrt{I - A^2})$. ∎

The proof of the following theorem is left to the reader (Problem 23).

Theorem VI.20 Let $\|\cdot\|_1$ be defined in $\mathscr{I}_1$ by $\|A\|_1 = \operatorname{tr}|A|$. Then $\mathscr{I}_1$ is a Banach space with norm $\|\cdot\|_1$ and $\|A\| \leq \|A\|_1$.

We note that $\mathscr{I}_1$ is *not* closed under the operator norm $\|\cdot\|$. The connection between the trace class operators and the compact operators is simple:

Theorem VI.21 Every $A \in \mathscr{I}_1$ is compact. A compact operator A is in $\mathscr{I}_1$ if and only if $\sum_{n=1}^{\infty} \lambda_n < \infty$ where $\{\lambda_n\}_{n=1}^{\infty}$ are the singular values of A.

Proof Since $A \in \mathscr{I}_1$, $|A|^2 \in \mathscr{I}_1$, so $\operatorname{tr}(|A|^2) = \sum_{n=1}^{\infty} \|A\varphi_n\|^2 < \infty$ for any orthonormal basis $\{\varphi_n\}_{n=1}^{\infty}$. Suppose $\psi \in [\varphi_1, \ldots, \varphi_N]^{\perp}$ and $\|\psi\| = 1$, then we have

$$\|A\psi\|^2 \leq \operatorname{tr}(|A|^2) - \sum_{n=1}^{N} \|A\varphi_n\|^2$$

since $\{\varphi_1, \varphi_2, \ldots, \varphi_N, \psi\}$ can always be completed to an orthonormal basis. Thus

$$\sup\{\|A\psi\| \mid \psi \in [\varphi_1, \ldots, \varphi_N]^{\perp}, \|\psi\| = 1\} \to 0 \quad \text{as} \quad N \to \infty$$

Therefore $\sum_{n=1}^{N} (\varphi_n, \cdot)A\varphi_n$ is norm convergent to A. Thus A is compact. The second part of the theorem follows easily from the canonical form derived in Theorem VI.17 (Problem 24). ∎

Corollary The finite rank operators are $\|\cdot\|_1$-dense in $\mathscr{I}_1$.

The second class of operators which we will discuss are the Hilbert-Schmidt operators, the analogue of $\mathscr{L}^2$.

Definition An operator $T \in \mathscr{L}(\mathscr{H})$ is called **Hilbert–Schmidt** if and only if $\operatorname{tr} T^*T < \infty$. The family of all Hilbert–Schmidt operators is denoted by $\mathscr{I}_2$.

By arguments analogous to those we used for $\mathscr{I}_1$, one can prove.

Theorem VI.22 (a) $\mathscr{I}_2$ is a $*$-ideal.

(b) If $A, B \in \mathscr{I}_2$, then for any orthonormal basis $\{\varphi_n\}$,

$$\sum_{n=1}^{\infty} (\varphi_n, A^*B\varphi_n)$$

is absolutely summable, and its limit, denoted by $(A, B)_2$, is independent of the orthonormal basis chosen.

(c) $\mathscr{I}_2$ with inner product $(\cdot, \cdot)_2$ is a Hilbert space.

(d) If $\|A\|_2 = \sqrt{(A, A)_2} = (\operatorname{tr}(A^*A))^{1/2}$, then

$$\|A\| \leq \|A\|_2 \leq \|A\|_1 \qquad \text{and} \qquad \|A\|_2 = \|A^*\|_2$$

(e) Every $A \in \mathscr{I}_2$ is compact and a compact operator, A, is in $\mathscr{I}_2$ if and only if $\sum_{n=1}^{\infty} \lambda_n^2 < \infty$ where λ_n are the singular values of A.

(f) The finite rank operators are $\|\cdot\|_2$-dense in $\mathscr{I}_2$.

(g) $A \in \mathscr{I}_2$ if and only if $\{\|A\varphi_n\|\} \in \ell_2$ for some orthonormal basis $\{\varphi_n\}$.

(h) $A \in \mathscr{I}_1$ if and only if $A = BC$ with B, C in $\mathscr{I}_2$.

We note that $\mathscr{I}_2$ is not $\|\cdot\|$-closed. The important fact about $\mathscr{I}_2$ is that when $\mathscr{H} = L^2(M, d\mu)$, $\mathscr{I}_2$ has a concrete realization.

Theorem VI.23 Let $\langle M, \mu \rangle$ be a measure space and $\mathscr{H} = L^2(M, d\mu)$. Then $A \in \mathscr{L}(\mathscr{H})$ is Hilbert–Schmidt if and only if there is a function

$$K \in L^2(M \times M, d\mu \otimes d\mu)$$

with

$$(Af)(x) = \int K(x, y) f(y)\, d\mu(y)$$

Moreover,

$$\|A\|_2^2 = \int |K(x, y)|^2\, d\mu(x)\, d\mu(y)$$

Proof Let $K \in L^2(M \times M, d\mu \otimes d\mu)$ and let A_K be the associated integral operator. It is easy to see (Problem 25) that A_K is a well-defined operator on $\mathscr{H}$ and that

$$\|A_K\| \leq \|K\|_{L^2} \tag{VI.8}$$

Let $\{\varphi_n\}_{n=1}^{\infty}$ be an orthonormal basis for $L^2(M, d\mu)$. Then $\{\varphi_n(x)\overline{\varphi_m(y)}\}_{n,m=1}^{\infty}$ is an orthonormal base for $L^2(M \times M, d\mu \otimes d\mu)$ so

$$K = \sum_{n,m=1}^{\infty} \alpha_{nm} \varphi_n(x)\overline{\varphi_m(y)}$$

Let

$$K_N = \sum_{n,m=1}^{N} \alpha_{n,m} \varphi_n(x)\overline{\varphi_m(y)}$$

Then each K_N is the integral kernel of a finite rank operator. In fact, $A_{K_N} = \sum_{n,m=1}^{N} \alpha_{nm}(\varphi_m, \cdot)\varphi_n$. Since $\|K_N - K\|_{L^2} \to 0$ we have $\|A_K - A_{K_N}\| \to 0$ as $N \to \infty$ by (VI.8). Thus A_K is compact and in fact

$$\operatorname{tr}(A_K^* A_K) = \sum_{n=1}^{\infty} \|A_K \varphi_n\|^2 = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} |\alpha_{nm}|^2 = \|K\|_{L^2}$$

Thus $A_K \in \mathscr{I}_2$ and $\|A_K\|_2 = \|K\|_{L^2}$.

We have shown that the map $K \to A_K$ is an isometry of $L^2(M \times M, d\mu \otimes d\mu)$ into $\mathscr{I}_2$, so its range is closed. But the finite rank operators clearly come from kernels and since they are dense in $\mathscr{I}_2$ the range of $K \mapsto A_K$ is all of $\mathscr{I}_2$. ∎

This theorem provides a simple sufficient condition for an operator to be compact and is therefore very useful. Notice that the condition is not necessary. Also, we have a sufficient condition for an operator on $\mathscr{H} = L^2(M, d\mu)$ to be an integral operator. This condition is also not necessary. Now, we return to defining the trace on $\mathscr{I}_1$.

Theorem VI.24 If $A \in \mathscr{I}_1$ and $\{\varphi_n\}_{n=1}^{\infty}$ is any orthonormal basis, then $\sum_{n=1}^{\infty} (\varphi_n, A\varphi_n)$ converges absolutely and the limit is independent of the choice of basis.

Proof We write $A = U|A|^{1/2}|A|^{1/2}$. Then

$$|(\varphi_n, A\varphi_n)| \leq \| |A|^{1/2} U^* \varphi_n \| \, \| |A|^{1/2} \varphi_n \|$$

Thus

$$\sum_{n=1}^{\infty} |(\varphi_n, A\varphi_n)| \leq \left(\sum_{n=1}^{\infty} \| |A|^{1/2} U^* \varphi_n \|^2 \right)^{1/2} \left(\sum_{n=1}^{\infty} \| |A|^{1/2} \varphi_n \|^2 \right)^{1/2}$$

so since $|A|^{1/2}U^*$ and $|A|^{1/2}$ are in $\mathscr{I}_2$, the sum converges. The proof of the independence of basis is identical to that for tr A when $A \geq 0$. ∎

Definition The map $\operatorname{tr}: \mathscr{I}_1 \to \mathbb{C}$ given by $\operatorname{tr} A = \sum_{n=1}^{\infty} (\varphi_n, A\varphi_n)$ where $\{\varphi_n\}$ is any orthonormal basis is called the **trace**.

We remark that it is not true that $\sum_{n=1}^{\infty} |(\varphi_n, A\varphi_n)| < \infty$ for some orthonormal basis implies $A \in \mathscr{I}_1$. For A to be in $\mathscr{I}_1$ the sum must be finite for all orthonormal bases. The spectral theorem which we will prove in the next chapter will tell us that any self-adjoint A can be written $A = A_+ - A_-$ where both A_+ and A_- are positive and $A_+ A_- = 0$. Not surprisingly, $A \in \mathscr{I}_1$ if and only if $\operatorname{tr}(A_+) < \infty$, $\operatorname{tr}(A_-) < \infty$ and in this case $\operatorname{tr} A = \operatorname{tr} A_+ - \operatorname{tr} A_-$. We collect the properties of the trace.

Theorem VI.25 (a) $\operatorname{tr}(\cdot)$ is linear.

(b) $\operatorname{tr} A^* = \overline{\operatorname{tr} A}$.

(c) $\operatorname{tr} AB = \operatorname{tr} BA$ if $A \in \mathscr{I}_1$ and $B \in \mathscr{L}(\mathscr{H})$.

Proof (a) and (b) are obvious. To prove (c) it is sufficient to consider the case where B is unitary since any bounded operator is the sum of four unitaries. In that case

$$\begin{aligned} \operatorname{tr} AB &= \sum_{n=1}^{\infty} (\varphi_n, AB\varphi_n) \\ &= \sum_{n=1}^{\infty} (B^*\psi_n, A\psi_n) \\ &= \sum_{n=1}^{\infty} (\psi_n, BA\psi_n) \\ &= \operatorname{tr} BA \end{aligned}$$

where $\psi_n = B\varphi_n$ for all n. ∎

If $A \in \mathscr{I}_1$, the map $B \mapsto \operatorname{tr} AB$ is a linear functional on $\mathscr{L}(\mathscr{H})$. These are not all the continuous linear functionals on $\mathscr{L}(\mathscr{H})$ but such functionals do yield the entire dual of $\operatorname{Com}(\mathscr{H})$, the compact operators. We can also hold $B \in \mathscr{L}(\mathscr{H})$ fixed and obtain a linear functional on $\mathscr{I}_1$ given by the map $A \mapsto \operatorname{tr} BA$. The set of these functionals is just the dual of $\mathscr{I}_1$ (with the operator norm topology). We state this as a theorem; the interested reader can follow the outline of the proof given in Problem 30.

Theorem VI.26 (a) $\mathscr{I}_1 = [\operatorname{Com}(\mathscr{H})]^*$. That is, the map $A \mapsto \operatorname{tr}(A\cdot)$ is an isometric isomorphism of $\mathscr{I}_1$ onto $[\operatorname{Com}(\mathscr{H})]^*$.

(b) $\mathscr{L}(\mathscr{H}) = \mathscr{I}_1^*$. That is, the map $B \mapsto \operatorname{tr}(B\cdot)$ is an isometric isomorphism of $\mathscr{L}(\mathscr{H})$ onto $\mathscr{I}_1^*$.

We now return to the distinction between the weak operator topology on $\mathscr{L}(\mathscr{H})$ (see Section VI.1) and the weak Banach space topology, i.e. the $\sigma(\mathscr{L}(\mathscr{H}), \mathscr{L}(\mathscr{H})^*)$ topology. If $\mathscr{F}$ is the family of finite rank operators, then $\mathscr{F} \subset \mathscr{I}_1$ and each $F \in \mathscr{F}$ can be realized as linear functional on $\mathscr{L}(\mathscr{H})$ via the dual action of $\mathscr{I}_1$ on $\mathscr{L}(\mathscr{H})$. The topology on $\mathscr{L}(\mathscr{H})$ generated by these functionals, that is, $\sigma(\mathscr{L}(\mathscr{H}), \mathscr{F})$ is just the weak operator topology. The set $\mathscr{F}$ is not closed in the $\mathscr{L}(\mathscr{H})^*$-norm. As a matter of fact, the $\mathscr{L}(\mathscr{H})^*$ norm on $\mathscr{F}$ is just $\|\cdot\|_1$ so the closure of $\mathscr{F}$ in this norm is just $\mathscr{I}_1$. The weak topology on $\mathscr{L}(\mathscr{H})$ generated by the functionals in $\mathscr{I}_1$, that is, $\sigma(\mathscr{L}(\mathscr{H}), \mathscr{I}_1)$, is called the **ultraweak** topology on $\mathscr{L}(\mathscr{H})$. Notice that it is stronger than the weak operator topology, since more functionals are required to be continuous, but weaker than the weak Banach space topology on $\mathscr{L}(\mathscr{H})$, since $\mathscr{I}_1$ is not the entire dual of $\mathscr{L}(\mathscr{H})$. In fact, since $\mathscr{L}(\mathscr{H}) = \mathscr{I}_1^*$, the ultraweak topology on $\mathscr{L}(\mathscr{H})$ is just the weak-$*$ topology. This realization of $\mathscr{L}(\mathscr{H})$ as the dual of the Banach space of linear functionals continuous in the $\sigma(\mathscr{L}(\mathscr{H}), \overline{\mathscr{F}})$ topology is valid for a larger class of algebras than just $\mathscr{L}(\mathscr{H})$. Problem 31 gives another example: the multiplication algebra L_∞ on L_2. We will study such algebras in detail in Chapter XVIII. We study the $\mathscr{I}_p$ spaces for $p \neq 1, 2, \infty$ in Sections IX.4 and XIII.17.

NOTES

Section VI.1 The reader may be bewildered by the many topologies we have introduced on $\mathscr{L}(\mathscr{H})$: the weak, strong, and uniform operator topologies, the weak Banach space topology, the ultraweak topology (Section VI.6). Later on we will even encounter the ultrastrong topology. Why is it necessary to introduce all these topologies? The answer is that many of the operators we are interested in are given as some sort of limit of simpler operators. It is important to know exactly what one means by "some sort" and to know what properties of the limiting operator follow from properties in the sequence, for example, the uniform limit of compact operators is compact. Furthermore, when one begins a problem one doesn't always know in what sense limits will exist, so it is useful to have a wide range of topologies at hand. In general it is the weak, strong, and uniform operator topologies which are important in Volumes I and II. The ultraweak and ultrastrong topologies will play a role when we deal with von Neumann algebras. The weak, strong, and ultrastrong operator topologies were introduced in J. von Neumann, "Zur Algebra der Functionaloperationen und Theorie der Normalen Operatoren," *Math. Ann.* **102** (1929–1930), 370–427.

Section VI.2 The spectral theorem for self-adjoint operators on finite dimensional vector spaces is nicely described in P. R. Halmos, *Finite Dimensional Vector Spaces*, Van Nostrand–Reinhold, Princeton, New Jersey, 1958.

Section VI.3 The definitions of various kinds of spectra will also be used for unbounded operators. Theorem VI.5 holds as long as we require that T be closed. If T is bounded it is, of course, automatically closed.

The theory of Banach space-valued analytic functions is described in great detail in *Functional Analysis and Semi-groups*, Amer. Math. Soc., Providence, Rhode Island, 1957, by E. Hille and R. S. Phillips. They also discuss the more difficult notion of analytic functions from one Banach space to another. A proof of Theorem VI.7 can be found in *Functional Analysis*, Academic Press, New York, 1965, by K. Yosida.

Some authors (for example: Yosida or Hille, Phillips) use the term "continuous spectrum" to denote any $\lambda \in \sigma(T)$ which is neither in the point spectrum, nor in the residual spectrum. Other authors (such as Kato or Riesz, Nagy) use the definition that we give in Section VII.2. One important distinction is that with our definition the continuous spectrum and the point spectrum need not be disjoint.

Section VI.4 The polar decomposition has a simple geometric meaning for linear transformations on $\mathbb{R}^n$. Any linear transformation A on $\mathbb{R}^n$ can be written as $A = OS$ where O is orthogonal and S is self-adjoint. By the spectral theorem, S can be thought of as a dilation, contraction, or annihilation in certain preferred orthogonal directions.

The notion of positivity has a natural generalization to operator algebras and will play an important role in our investigations in Volume III.

The statement that the triangle inequality fails for $|\cdot|$, that is, $|A + B|$ may *not* be less than or equal to $|A| + |B|$ (see Problem 16) is a statement that $f(x) = |x|$ is not a convex *operator-valued* function, that is, for $0 \leq t \leq 1$, $f(tA + (1-t)B) \leq tf(A) + (1-t)f(B)$ can be false for general operators A and B despite the fact that $f(tx - (1-t)y) \leq tf(x) + (1-t)f(y)$ is true for x and y real and $0 \leq t \leq 1$. Exactly which matrix and operator valued functions are convex has been studied in: F. Krauss, "Über konvexe Matrixfunktionen," *Math. Z.* **41** (1936) 18–42, and J. Bendat and S. Sherman, "Monotone and Convex Operator Functions," *Trans. Amer. Math. Soc.* **79** (1955), 58–71.

Section VI.5 The proof of the second part of Theorem VI.12 can be found in Yosida's book; it is a nice application of the Ascoli–Arzela and Alaoglu theorems (see also Problem 36).

In a very real sense, the theory of compact operators goes back to Fredholm's great paper on integral operators, "Sur une class d'équations fonctionnelles," *Acta Math.* **27** (1903), 365–390. Fredholm considered solving equations of the form

$$f(x) = g(x) + \lambda \int_a^b K(x, y) f(y)\, dy$$

where g and K are given continuous functions and $-\infty < a < b < \infty$. Fredholm showed that there exists an explicit entire function $d(\lambda)$, not identically zero, and an explicit function $D_\lambda(x, y)$, entire in λ and continuous in x and y, so that if $d(\lambda) \neq 0$, then $f(x) = g(x) + d(\lambda)^{-1} \int_a^b D_\lambda(x, y) g(y)\, dy$ solves the equation. Moreover, he showed that when $d(\lambda) = 0$, then

$$f(x) = \lambda \int_a^b K(x, y) f(y)\, dy$$

has a solution $f \neq 0$. Fredholm thus had Theorem VI.15 and the preceding corollary in this special case. Readable expositions of the Fredholm theory may be found in W. Lovitt: *Linear Integral Equations*, Dover, New York (reprinted 1950; original edition, McGraw-Hill,

New York, 1926), and F. Smithies, *Integral Equations*, Cambridge Univ. Press, London and New York, 1958.

Fredholm's work produced considerable interest among Hilbert and his school and led to the abstraction of many notions we now associate with Hilbert space theory. Hilbert first defined completely continuous operators in a manner whose modern form would be the criterion of Theorem VI.11: D. Hilbert, "Grundzüge einer allgemeinen Theorie der linearen Integralgleichungen, I–VI," *Nachr. Akad. Wiss. Göttingen Math.-Phys. Kl.* 49–91 (1904), 213–259, 307–388 (1905); 157–222, 439–480 (1906); 355–417 (1910); esp. IV. The extension of the notion of compact operator to arbitrary Banach spaces by the precompactness criteria is due to F. Riesz "Über lineare Functionalgleichungen," *Acta. Math.* 41 (1918), 71–98.

Theorem VI.12b is due to J. Schauder: "Über lineare, vollstetige Functionaloperationen," *Studia Math.* 2 (1930), 183–196.

The idea of using Theorem IV.13 to develop the general theory is due to E. Schmidt, "Auflösung der allgemeinen linearen Integralgleichung," *Math. Ann.* 64 (1907), 161–174. While it is true that compact operators in most explicit Banach spaces are norm limits of finite rank operators, there are Banach spaces where this is false. The earliest examples were constructed by P. Enflo. For extensive discussion, see M. M. Day, *Normed Linear Spaces*, Springer, Berlin, 1973, and J. Lindenstrauss and L. Tzafriri, *Classical Banach Spaces*, Springer Lecture Notes in Math 388, Springer-Verlag, 1973.

Theorem VI.14, its corollary, and Theorem VI.15 hold in an arbitrary Banach space. For their proof in that case, see N. Dunford and J. Schwartz, *Linear Operators*, Vol. I. Wiley (Interscience), 1958. Our technique of proof for Theorem VI.14 is taken from a technical appendix in W. Hunziker, "On the Spectra of Schrödinger Multiparticle Hamiltonians," *Helv. Phys. Acta.* 39 (1966), 451–462. A similar approach can be found in an appendix of G. Tiktopolous, "Analytic Continuation in Complex Angular Momentum and Integral Equations," *Phys. Rev.* 133B (1964), 1231–1238. One part of Theorem VI.14 is not proven in the general case in Dunford–Schwartz; a discussion of this extra point can be found in S. Steinberg, "Meromorphic Families of Compact Operators," *Arch. Rat. Mech. Anal.* 31 (1968), 372–379. For extensions to locally convex spaces, see J. Leray, "Valeurs propres et vecteurs propres d'un endomorphisme conplètement continu d'un espace vectoriel à voisinages convexes," *Acta Sci. Math. Szcg.* 12, Part B, (1950), 177–186. Theorem VI.15 was first proven by Riesz and Schauder in the above cited works (Schauder filled in some details for the general case) and Theorem VI.16 is due to Hilbert and Schmidt in the aforementioned papers.

For a discussion of the use of integral equations in the solution of Dirichlet problem, see *Boundary Value Problems of Mathematical Physics*, Vol. 2, (especially sections 6.4 and 6.5), Macmillan, New York, 1968, by Ivor Stakgold and Volume II of R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Wiley (Interscience).

Section VI.6 For a discussion on $\mathcal{I}_1$, $\mathcal{I}_2$, and the $\mathcal{I}_p$ analogues, see R. Schatten, *Norm Ideals of Completely Continuous Operators*, Springer–Verlag, Berlin and New York, 1960. $\mathcal{I}_p$ is defined as those A with $\mathrm{Tr}(|A|^p) < \infty$ and is equivalently those compact operators with $\sum |\lambda_n|^p < \infty$. For further discussion, see Sections IX.4 and XIII.17.

These norm ideals have been extended to other situations with traces (von Neumann algebras) and more general settings in a manner emphasizing the analogy with L^p by I. Segal: "A Non-Commutative Extension of Abstract Integration," *Ann. Math.* 57 (1953), 401–457; 58 (1953), 595–596, and R. A. Kunze, "L_p Fourier Transforms on Locally Compact Unimodular Groups," *Trans. Amer. Math. Soc.* 89 (1958), 519.

PROBLEMS

†1. **Prove that the weak operator topology is weaker than the strong operator topology** which is weaker than the uniform operator topology.

†2. Prove the statements in the example in Section VI.1.

3. (a) Let X and Y be Banach spaces. Prove that if $T_n \in \mathscr{L}(X, Y)$ and $\{T_n x\}$ is a Cauchy sequence for each $x \in X$, then there exists a $T \in \mathscr{L}(X, Y)$ so that $T_n \to T$ strongly.
*(b) Is the theorem in (a) true if T_n is replaced by a net T_α?

4. (a) Let X and Y be Banach spaces. Prove that a theorem for $\mathscr{L}(X, Y)$ analogous to Theorem VI.1 holds if Y is weakly sequentially complete (which means that every weakly Cauchy sequence has a weak limit.)
(b) **Prove that if a Banach space is reflexive, then it is weakly sequentially complete.**

5. (a) Let T_t be the operator $T_t\colon \varphi(x) \to \varphi(x + t)$ on $L^2(\mathbb{R})$. What is the norm of T_t? To what operator does T_t converge as $t \to \infty$ and in what topology?
(b) Answer the same question for T_t if the Hilbert space is $L^2(\mathbb{R}, e^{-x^2}\,dx)$.

6. (a) Let $\mathscr{H}$ be an infinite dimensional Hilbert space. Suppose $\psi_1, \ldots, \psi_n$ orthonormal are given and that ε, ψ are given. Show there are A and B with $\|A\psi_i\| < \varepsilon$, $\|B\psi_i\| = \varepsilon$; $i = 1, \ldots, n$, but that $\|AB\psi\| > 1$.
(b) Prove that multiplication from $\mathscr{L}(\mathscr{H}) \times \mathscr{L}(\mathscr{H}) \to \mathscr{L}(\mathscr{H})$ is not jointly continuous when $\mathscr{L}(\mathscr{H})$ is given the strong topology.
(c) Suppose $\{A_\alpha\}_{\alpha \in I}$ and $\{B_\alpha\}_{\alpha \in I}$ are *nets*. Let $A_\alpha^* \xrightarrow{s} A^*$, $B_\alpha \xrightarrow{s} B$. Prove that $A_\alpha B_\alpha \xrightarrow{w} AB$.
(d) Let A_n, B_n be *sequences* so that $A_n \xrightarrow{s} A$, $B_n \xrightarrow{s} B$. Prove that $A_n B_n \xrightarrow{s} AB$.
(e) Let A_n, B_n be *sequences* so that $A_n \xrightarrow{w} A$, $B_n \xrightarrow{w} B$. Give an example where $A_n B_n \xrightarrow{w} AB$ is *false*.

7. Give an example to show that the range of a bounded operator need not be closed. Prove that if T is bounded, everywhere defined, and an isometry, then Ran T is closed.

†8. (a) Let A be a self-adjoint bounded operator on a Hilbert space. Prove that the eigenvalues of A are real and that the eigenvectors corresponding to distinct eigenvalues are orthogonal.
(b) From the proof of Theorem VI.8 derive a universal (but λ-dependent) bound for the norm of the resolvent of a self-adjoint operator at a nonreal $\lambda \in \mathbb{C}$.

9. (a) Let A be a self-adjoint operator on a Hilbert space, $\mathscr{H}$. Prove that

$$\|A\| = \sup_{\|x\| = 1} |(Ax, x)|$$

Hint: First note that

$$\operatorname{Re}(\psi, A\phi) = \tfrac{1}{4}[(\psi + \phi, A(\psi + \phi)) - (\psi - \phi, A(\psi - \phi))]$$

Then using

$$|(\eta, A\eta)| \leq \|\eta\|^2 \sup_{\|\eta\| = 1} |(\eta, A\eta)|$$

and the parallelogram law, prove that

$$|(\psi, A\phi)| \leq \sup_{\|\eta\| = 1} |(\eta, A\eta)|$$

if $\|\varphi\| = \|\psi\| = 1$.

(b) Find an example which shows that the conclusion of (a) need not be true if A is not self-adjoint.

10. Show that the spectral radius of the Volterra integral operator

$$(Tf)(x) = \int_0^x f(y)\,dy$$

as a map on $C[0, 1]$ is equal to zero. What is the norm of T?

†*11.* Let $T \in \mathscr{L}(X)$. Prove that $\lim_{n\to\infty} \|T^n\|^{1/n}$ exists and is equal to $\inf_n \|T^n\|^{1/n}$ as follows:
(a) Set $a_n = \log \|T^n\|$ and prove that $a_{m+n} \leq a_m + a_n$.
(b) For a fixed positive integer m set $n = mq + r$ where q and r are positive integers and $0 \leq r \leq m - 1$. Using (a) conclude that

$$\overline{\lim_n} \frac{a_n}{n} \leq \frac{a_m}{m}$$

(c) Prove that $\lim_{n\to\infty} a_n/n = \inf_n a_n/n$ and thus the desired equality.

†*12.* Prove the proposition at the end of Section VI.3.

13. (a) Give an example which shows that a linear transformation on $\mathbb{C}^n$ can be positive without all the entries in a given matrix representation being positive.
*(b) Derive a necessary and sufficient condition for a $n \times n$ matrix to be positive.

14. (a) Prove that if $A_n \geq 0$, $A_n \to A$ in norm, then $\sqrt{A_n} \to \sqrt{A}$ norm.
(b) Suppose $A_n \to A$ strongly for a sequence $\{A_n\}$. Prove that $\sqrt{A_n} \to \sqrt{A}$ strongly.

15. (a) Let $A_n \to A$ in norm. Prove that $|A_n| \to |A|$ in norm.
(b) Suppose $A_n \to A$ and $A_n^* \to A^*$ strongly where A_n is a sequence. Prove that $|A_n| \to |A|$ strongly.
(c) Find an example which shows that $|\cdot|$ is not weakly continuous on $\mathscr{L}(\mathscr{H})$.

16. Let $\sigma_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$, $\sigma_1 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$. Prove that it is false that

$$|(\sigma_3 + 1) + (\sigma_1 - 1)| \leq |(\sigma_3 + 1)| + |(\sigma_1 - 1)|$$

Remark: This example is due to E. Nelson.

17. Show that it is not necessarily true that

$$\| \,|A| - |B|\, \| \leq \|A - B\|$$

(*Hint*: See Problem 16.)

†*18.* (a) Prove the proposition preceding Theorem VI.10.
(b) Prove the uniqueness in Theorem VI.10.

19. Write the matrix $\left(\begin{smallmatrix} -\frac{1}{2} & -2 \\ 1 & 1 \end{smallmatrix}\right)$ as the product of a rotation and a positive symmetric matrix.

**20.* Suppose that X is a reflexive Banach space and that T: $X \to X$ a bounded linear operator. Prove that if T takes weakly convergent sequences into norm convergent sequences, then T is compact.

†*21.* Complete the proof of Theorem VI.14 by extending the result to all of D.

22. Using the Stone–Weierstrass theorem prove that every Fredholm integral operator on $C[a, b]$

$$(Tf)(x) = \int_a^b K(x, y) f(y)\, dy$$

where K is continuous, is a norm limit of operators of finite rank.

†23. (a) Prove that $\|A\| \leq \|A\|_1$.
(b) Suppose $\{A_n\}$ is an $\|\cdot\|_1$-Cauchy sequence. Show that $\{A_n\}$ has a $\|\cdot\|$-limit A and that $\operatorname{tr}|A| < \infty$. Then conclude the proof of Theorem VI.20 by showing that A is the $\|\cdot\|_1$-limit of $\{A_n\}$.

†24. (a) Use the canonical form given by Theorem VI.17 to prove the second statement in Theorem VI.21.
(b) Prove the corollary to Theorem VI.21.

†25. Let $K \in L^2(M \times M, d\mu \otimes d\mu)$ and let A_K be the integral operator

$$(A_K \varphi)(x) = \int_M K(x, y) \varphi(y)\, d\mu(y)$$

Prove that A_K is well defined and $\|A_K\| \leq \|K\|_{L^2}$.

26. (a) Prove that if $\sum_{n=1}^{\infty} |(A\varphi_n, \varphi_n)| < \infty$ for all orthonormal bases, then $A \in \mathscr{I}_1$.
(b) Find an $A \notin \mathscr{I}_1$ so that $\sum_{n=1}^{\infty} |(A\varphi_n, \varphi_n)| < \infty$ for some fixed orthonormal basis.

27. Prove that $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ if $A, B \in \mathscr{I}_2$.

28. Prove that (a) $\|AB\|_1 \leq \|A\|\ \|B\|_1$
(b) $\|AB\|_2 \leq \|A\|\ \|B\|_2$
(c) $\|AB\|_1 \leq \|A\|_2 \|B\|_2$

·29. Prove that $A \in \mathscr{I}_1$ if and only if $A = BC$ with B and C in $\mathscr{I}_2$.

·30. The goal of this problem is to prove Theorem VI.26.
(a) Let f be a bounded linear functional on $\operatorname{Com}(\mathscr{H})$. Let $(\psi, \cdot)\phi$ be the operator on $\mathscr{H}$ which takes η into $(\psi, \eta)\phi$. Show that there is a unique bounded linear operator, B, with

$$(\psi, B\phi) = f[(\psi, \cdot)\phi]$$

(b) Using the fact that

$$\sum_{n=1}^{N} (\phi_n, |B|\phi_n) = f\left[\sum_{n=1}^{N} (U\phi_n, \cdot)\phi_n\right]$$

prove that $B \in \mathscr{I}_1$ and $\|B\|_1 \leq \|f\|_{\operatorname{Com}(\mathscr{H})^*}$.
(c) Prove that $A \mapsto \operatorname{tr}(BA)$ is a bounded linear functional on $\operatorname{Com}(\mathscr{H})$ which is in fact equal to $f(\cdot)$.
(d) Prove that $\|B\|_1 = \|f\|_{\operatorname{Com}(\mathscr{H})^*}$.
(e) Let g be a bounded linear functional on $\mathscr{I}_1$. Show that there is a unique bounded linear operator, B, with

$$(\psi, B\phi) = g[(\psi, \cdot)\phi]$$

(f) Prove that $A \mapsto \operatorname{tr}(BA)$ is a bounded linear functional on $\mathscr{I}_1$ which agrees with g and that $\|g\|_{\mathscr{I}_1^*} = \|B\|$.

31. Let $\langle M, \mu\rangle$ be a measure space and let $L^\infty(M, d\mu)$ act on $\mathscr{H} = L^2(M, d\mu)$ by

$$(T_f\varphi)(x) = f(x)\varphi(x)$$

Prove that the topology on L^∞ induced by the weak operator topology on $\mathscr{L}(\mathscr{H})$ is identical to the weak-* topology induced on L^∞ by L^1.

32. Let $C[0, 1]$ act on $L^2(0, 1)$ as in Problem 31. Find a sequence in $C[0, 1]$ convergent in the weak operator topology on $C[0, 1]$ to $f \in C[0, 1]$ which is not convergent in the weak Banach space topology on $C[0, 1]$.

33. Consider $\mathscr{I}_2$ as a Hilbert space with inner product $(A, B)_2 = \operatorname{tr}(A^*B)$. Let $A \mapsto L_A$ and $A \mapsto R_A$ be the maps of $\mathscr{L}(\mathscr{H})$ into $\mathscr{L}(\mathscr{I}_2)$ given by

$$L_A(B) = AB, \qquad R_A(B) = BA^*$$

(a) Prove that $A \mapsto L_A$ is a homomorphism of $\mathscr{L}(\mathscr{H})$ into $\mathscr{L}(\mathscr{I}_2)$.
(b) Prove that $A \mapsto R_A$ is a conjugate linear homomorphism of $\mathscr{L}(\mathscr{H})$ into $\mathscr{L}(\mathscr{I}_2)$.
(c) Suppose that $C \in \mathscr{L}(\mathscr{I}_2)$ and obeys $CL_A = L_A C$ for all $A \in \mathscr{L}(\mathscr{H})$. Prove that $C = R_B$ for some $B \in \mathscr{L}(\mathscr{H})$.

***34.** Show that in a Hilbert space, a map $T: \mathscr{H} \to \mathscr{H}$ is continuous if the domain is given the weak topology and the range the norm topology (that is, $x_\alpha \overset{w}{\to} x$ implies $Tx_\alpha \overset{\|\cdot\|}{\to} Tx$ for arbitrary *nets*) if and only if T has finite rank! (Compare with Theorem VI.11.)

35. (a) Suppose T is an operator in $\mathscr{L}(\mathscr{H})$ so that $x_n \overset{\|\cdot\|}{\to} x$ implies $Tx_n \overset{w}{\to} Tx$. Prove T is bounded (so $Tx_n \overset{\|\cdot\|}{\to} Tx$).
(b) Identify the continuous linear maps of $\mathscr{L}(\mathscr{H})$ into itself if both the domain and range are given the weak topology.

36. Use (c) of Theorem VI.12 and the polar decomposition to prove (b) of Theorem VI.12 when $X = Y$ is a Hilbert space.

†*37.* Prove part (c) of Theorem VI.12.

38. Let P and Q be orthogonal projections onto subspaces $\mathscr{M}$ and $\mathscr{N}$ in a Hilbert space $\mathscr{H}$. Suppose that $PQ = QP$.
(a) Prove $1 - P, 1 - Q, PQ, P + Q - PQ$ and $P + Q - 2PQ$ are orthogonal projections.
(b) How are the ranges of the projections in (a) related to $\mathscr{M}$ and $\mathscr{N}$.

***39.** Let P and Q be orthogonal projections onto subspaces $\mathscr{M}$ and $\mathscr{N}$ in a Hilbert space $\mathscr{H}$. Prove that s-lim$_{n\to\infty} (PQ)^n$ exists and is the orthogonal projection onto $\mathscr{M} \cap \mathscr{N}$.

***40.** Let $\mathscr{I}$ be a norm closed ideal in $\mathscr{L}(\mathscr{H})$, $\mathscr{I} \neq 0$. Prove $\operatorname{Com}(\mathscr{H}) \subset \mathscr{I}$ by proving that any finite rank operator is in $\mathscr{I}$.

Remark: We will see (Chapter VII, Problem 31) that the only norm closed ideals when $\mathscr{H}$ is separable are $\{0\}$, $\operatorname{Com}(\mathscr{H})$, $\mathscr{L}(\mathscr{H})$.

41. Find a projection on $\mathbb{R}^2$ which is not an orthogonal projection.

42. Let $A \in \mathscr{L}(X)$. Prove that the set of λ such that λ is in $\sigma(A)$ but not an eigenvalue and $\operatorname{Ran}(\lambda I - A)$ is closed but not all of X is a open subset of $\mathbb{C}$.

43. Let M and N be subspaces of a Banach space X such that $M + N = X$ and $M \cap N = \{0\}$. Let P be the projection of X onto M. Prove that P is bounded if and only if *both* M and N are closed.

44. (a) Define the numerical range, $N(T)$, of a bounded operator, T, on a Hilbert space, $\mathscr{H}$, by $N(T) = \{(\psi, T\psi) | \psi \in \mathscr{H}, \ \|\psi\| = 1\}$. Prove that $\sigma(T) \subset \overline{N(T)}$. (Hint: First show that if λ is an eigenvalue of T or T^*, then $\lambda \in N(T)$; then show that if $\lambda \in \sigma(T)$ and λ is not an eigenvalue of T or T^*, we can find $\psi_n \in \mathscr{H}$ so that $\|(T - \lambda)\psi_n\| \to 0$.)

(b) Find an example where $N(T)$ is not closed and $\sigma(T) \not\subset N(T)$.

(c) Find an example where $\sigma(T) \neq N(T) = \overline{N(T)}$.

Remark: There is a deep result of Hausdorff that $N(T)$ is convex.

45. (a) Let $\{\phi_n\}_{n=1}^{\infty}$ be an orthonormal basis for a Hilbert space $\mathscr{H}$. Let A be an operator with

$$\sup_{\substack{\psi \in \{\phi_1, \ldots, \phi_n\}^{\perp} \\ \|\psi\| = 1}} \|A\psi\| \to 0 \qquad \text{as} \quad n \to \infty.$$

Prove that A is compact.

(b) Let $\{\phi_n\}_{n=1}^{\infty}$ be any orthonormal basis for a Hilbert space $\mathscr{H}$ and let A be compact. Prove that

$$\sup_{\psi \in \{\phi_1, \ldots, \phi_n\}^{\perp}} \|A\psi\| \to 0 \qquad \text{as} \quad n \to \infty.$$

46. (a) Let $A \geq 0$ with A compact. Prove that $A^{1/2}$ is compact. (Hint: Use Problem 45.)

(b) Let $0 \leq A \leq B$. Prove that A is compact if B is compact. (Hint: Prove that $A^{1/2}$ is compact using Problem 45 and part (a).)

47. Let $\mathscr{H}$ and $\mathscr{H}'$ be two Hilbert spaces. If T is a bounded linear map from $\mathscr{H}$ to $\mathscr{H}'$ we define $T^*: \mathscr{H}' \to \mathscr{H}$ by $(T^*\psi, \phi)_{\mathscr{H}} = (\psi, T\phi)$. T is called *Hilbert–Schmidt* if and only if $T^*T: \mathscr{H} \to \mathscr{H}$ is trace class. Let T be Hilbert–Schmidt. Prove that there are real numbers, $\lambda_n > 0$, and orthonormal sets $\{\phi_n\}_{n=1}^{N} \subset \mathscr{H}$, $\{\psi_n\}_{n=1}^{N} \in \mathscr{H}'$ so that

$$T\phi = \sum_{n=1}^{N} \lambda_n (\phi_n, \phi)\psi_n$$

48. Let $\mathscr{H}$ and $\mathscr{H}'$ be the two Hilbert spaces and let $\mathscr{I}_2(\mathscr{H}, \mathscr{H}')$ denote the Hilbert–Schmidt operators from $\mathscr{H}$ to $\mathscr{H}'$.

(a) Prove that $\mathscr{I}_2(\mathscr{H}, \mathscr{H}')$ with the inner product

$$(S, T) = \mathrm{Tr}_{\mathscr{H}}(S^*T)$$

is a Hilbert space.

(b) Given $\psi \in \mathscr{H}$, $\phi \in \mathscr{H}'$ define $I(\psi, \phi) \in \mathscr{I}_2(\mathscr{H}^*, \mathscr{H}')$ by $I(\psi, \phi)\ell = \ell(\psi)\phi$ for any $\ell \in \mathscr{H}^*$. Prove that the map J, taking $\psi \otimes \phi$ into $I(\psi, \phi)$, is well defined and extends to an isometry of $\mathscr{H} \otimes \mathscr{H}'$ and $\mathscr{I}_2(\mathscr{H}^*, \mathscr{H}')$.

(c) Given $\eta \in \mathscr{H} \otimes \mathscr{H}'$ show that there exist reals, $\lambda_n > 0$, and orthonormal sets $\{\phi_n\}_{n=1}^{N} \subset \mathscr{H}$, $\{\psi_n\}_{n=1}^{N} \subset \mathscr{H}'$ with N finite or infinite, so that

$$\sum_{n=1}^{N} |\lambda_n|^2 = \|\eta\|^2 \qquad \text{and} \qquad \sum_{n=1}^{N} \lambda_n \phi_n \otimes \psi_n = \eta.$$

VII: The Spectral Theorem

Mathematical proofs, like diamonds, are hard as well as clear, and will be touched with nothing but strict reasoning. *John Locke in* ***Second Reply to the Bishop of Worcester***

VII.1 The continuous functional calculus

In this chapter, we will discuss the spectral theorem in its many guises. This structure theorem is a concrete description of all self-adjoint operators. There are several apparently distinct formulations of the spectral theorem. In some sense they are all equivalent.

The form we prefer says that every bounded self-adjoint operator is a multiplication operator. (We emphasize the word bounded since we will deal extensively with unbounded self-adjoint operators in the next chapter; there is a spectral theorem for unbounded operators which we discuss in Section VIII.3.) This means that given a bounded self-adjoint operator on a Hilbert space $\mathscr{H}$, we can always find a measure μ on a measure space M and a unitary operator $U: \mathscr{H} \to L^2(M, d\mu)$ so that

$$(UAU^{-1}f)(x) = F(x)f(x)$$

for some bounded real-valued measurable function F on M.

This is clearly a generalization of the finite-dimensional theorem, which says any self-adjoint $n \times n$ matrix can be diagonalized, or in an abstract form: Given self-adjoint operator A on an n-dimensional complex space V,

there is a unitary operator $U: V \to \mathbb{C}^n$ and real numbers $\lambda_1, \ldots, \lambda_n$ so that

$$(UAU^{-1}f)_i = \lambda_i f_i$$

for each $f = \langle f_1, \ldots, f_n \rangle$ in $\mathbb{C}^n$.

In practice, M will be a union of copies of $\mathbb{R}$ and F will be x, so the core of the proof of the theorem will be the construction of certain measures. This will be done in Section VII.2 by using the Riesz–Markov theorem. Our goal in this section will be to make sense out of $f(A)$, for f a continuous function. In the next section, we will consider the measures defined by the functionals $f \mapsto \langle \psi, f(A)\psi \rangle$ for fixed $\psi \in \mathscr{H}$.

Given a fixed operator A, for which f can we define $f(A)$? First, suppose that A is an arbitrary bounded operator. If $f(x) = \sum_{n=1}^{N} a_n x^n$ is a polynomial, we want $f(A) = \sum_{n=1}^{N} a_n A^n$. Suppose that $f(x) = \sum_{n=0}^{\infty} c_n x^n$ is a power series with radius of convergence R. If $\|A\| < R$, then $\sum_{n=0}^{\infty} c_n A^n$ converges in $\mathscr{L}(\mathscr{H})$ so it is natural to set $f(A) = \sum_{n=0}^{\infty} c_n A^n$. In this last case, f was a function analytic in a domain including all of $\sigma(A)$. In general, one can make a reasonable definition for $f(A)$ if f is analytic in a neighborhood of $\sigma(A)$ (see the Notes).

The functional calculus we have talked about thus far works for any operator in any Banach space. The special property of self-adjoint operators (or more generally normal operators; see Problems 3, 5) is that $\|P(A)\| = \sup_{\lambda \in \sigma(A)} |P(\lambda)|$ for any polynomial P, so that one can use the B.L.T. theorem to extend the functional calculus to continuous functions. Our major goal in this section is the proof of:

Theorem VII.1 (continuous functional calculus) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Then there is a *unique* map $\phi: C(\sigma(A)) \to \mathscr{L}(\mathscr{H})$ with the following properties:

(a) ϕ is an algebraic $*$-homomorphism, that is,

$$\phi(fg) = \phi(f)\phi(g) \qquad \phi(\lambda f) = \lambda\phi(f)$$
$$\phi(1) = I \qquad \phi(\bar{f}) = \phi(f)^*$$

(b) ϕ is continuous, that is, $\|\phi(f)\|_{\mathscr{L}(\mathscr{H})} \leq C\|f\|_\infty$.

(c) Let f be the function $f(x) = x$; then $\phi(f) = A$.

Moreover, ϕ has the additional properties:

(d) If $A\psi = \lambda\psi$, then $\phi(f)\psi = f(\lambda)\psi$.

(e) $\sigma[\phi(f)] = \{f(\lambda) \mid \lambda \in \sigma(A)\}$ [spectral mapping theorem].

(f) If $f \geq 0$, then $\phi(f) \geq 0$.

(g) $\|\phi(f)\| = \|f\|_\infty$ [this strengthens (b)].

We sometimes write $\phi_A(f)$ or $f(A)$ for $\phi(f)$ to emphasize the dependence on A.

The idea of the proof which we give below is quite simple. (a) and (c) uniquely determine $\phi(P)$ for any polynomial $P(x)$. By the Weierstrass theorem, the set of polynomials is dense in $C(\sigma(A))$ so the heart of the proof is showing that

$$\|P(A)\|_{\mathscr{L}(\mathscr{H})} = \|P(x)\|_{C(\sigma(A))} \equiv \sup_{\lambda \in \sigma(A)} |P(\lambda)|$$

The existence and uniqueness of ϕ then follow from the B.L.T. theorem.

To prove the crucial equality, we first prove a special case of (e) (which holds for arbitrary bounded operators):

Lemma 1 Let $P(x) = \sum_{n=0}^{N} a_n x^n$. Let $P(A) = \sum_{n=0}^{N} a_n A^n$. Then

$$\sigma(P(A)) = \{P(\lambda) \mid \lambda \in \sigma(A)\}$$

Proof Let $\lambda \in \sigma(A)$. Since $x = \lambda$ is a root of $P(x) - P(\lambda)$, we have $P(x) - P(\lambda) = (x - \lambda)Q(x)$, so $P(A) - P(\lambda) = (A - \lambda)Q(A)$. Since $(A - \lambda)$ has no inverse neither does $P(A) - P(\lambda)$, that is, $P(\lambda) \in \sigma(P(A))$.

Conversely, let $\mu \in \sigma(P(A))$ and let $\lambda_1, \ldots, \lambda_n$ be the roots of $P(x) - \mu$, that is, $P(x) - \mu = a(x - \lambda_1) \cdots (x - \lambda_n)$. If $\lambda_1, \ldots, \lambda_n \notin \sigma(A)$, then

$$(P(A) - \mu)^{-1} = a^{-1}(A - \lambda_1)^{-1} \cdots (A - \lambda_n)^{-1}$$

so we conclude that some $\lambda_i \in \sigma(A)$, that is, $\mu = P(\lambda)$ for some $\lambda \in \sigma(A)$. ∎

Lemma 2 Let A be a bounded self-adjoint operator. Then

$$\|P(A)\| = \sup_{\lambda \in \sigma(A)} |P(\lambda)|$$

Proof

$$\begin{aligned}
\|P(A)\|^2 &= \|P(A)^* P(A)\| \\
&= \|(\bar{P}P)(A)\| \\
&= \sup_{\lambda \in \sigma(\bar{P}P(A))} |\lambda| \qquad \text{(by Theorem VI.6)} \\
&= \sup_{\lambda \in \sigma(A)} |\bar{P}P(\lambda)| \qquad \text{(by Lemma 1)} \\
&= \left(\sup_{\lambda \in \sigma(A)} |P(\lambda)| \right)^2
\end{aligned}$$

∎

Proof of Theorem VII.1 Let $\phi(P) = P(A)$. Then $\|\phi(P)\|_{\mathscr{L}(\mathscr{H})} = \|P\|_{C(\sigma(A))}$ so ϕ has a unique linear extension to the closure of the polynomials in $C(\sigma(A))$. Since the polynomials are an algebra containing 1, containing complex

conjugates, and separating points, this closure is all of $C(\sigma(A))$. Properties (a), (b), (c), (g) are obvious and if $\tilde{\phi}$ obeys (a), (b), (c) it agrees with ϕ on polynomials and thus by continuity on $C(\sigma(A))$. To prove (d), note that $\phi(P)\psi = P(\lambda)\psi$ and apply continuity. To prove (f), notice that if $f \geq 0$, then $f = g^2$ with g real and $g \in C(\sigma(A))$. Thus $\phi(f) = \phi(g)^2$ with $\phi(g)$ self-adjoint, so $\phi(f) \geq 0$. (e) is left for the reader (Problem 8). ∎

Before turning to some examples, we make several remarks:

(1) $\phi(f) \geq 0$ if and only if $f \geq 0$ (Problem 9).

(2) Since $fg = gf$ for all f, g, $\{f(A) \mid f \in C(\sigma(A))\}$ forms an abelian algebra closed under adjoints. Since $\|f(A)\| = \|f\|_\infty$ and $C(\sigma(A))$ is complete, $\{f(A) \mid f \in C(\sigma(A))\}$ is norm-closed. It is thus an **abelian C^* algebra** of operators.

(3) Ran ϕ is actually the **C^* algebra generated by A**, that is, the smallest C^*-algebra containing A (Problem 10).

(4) This result, that $C(\sigma(A))$ and the C^*-algebra generated by A are isometrically isomorphic, is actually a special case of the "commutative Gelfand–Naimark theorem" which we discuss in Chapter XV.

(5) (b) actually follows from (a) and abstract nonsense (Problem 11). Thus (a) and (c) alone determine ϕ uniquely.

Finally, we consider two specific examples of $\phi(f)$:

Example 1 As a corollary, we have a new proof of the existence half of the square-root lemma (Theorem VI.9) for if $A \geq 0$, then $\sigma(A) \subset [0, \infty)$ (Problem 12). If $f(x) = x^{1/2}$, then $f(A)^2 = A$.

Example 2 From (g) of Theorem VII.1 we see that $\|(A - \lambda)^{-1}\| = [\text{dist}(\lambda, \sigma(A))]^{-1}$ if A is bounded, self-adjoint, and $\lambda \notin \sigma(A)$.

VII.2 The spectral measures

We are now ready to introduce the measures we have anticipated so often before. Let us fix A, a bounded self-adjoint operator. Let $\psi \in \mathcal{H}$. Then $f \mapsto (\psi, f(A)\psi)$ is a positive linear functional on $C(\sigma(A))$. Thus, by the Riesz–Markov theorem (Theorem IV.14), there is a unique measure μ_ψ on the compact set $\sigma(A)$ with $(\psi, f(A)\psi) = \int_{\sigma(A)} f(\lambda)\, d\mu_\psi$.

Definition The measure μ_ψ is called the **spectral measure associated with the vector** ψ.

The first and simplest application of the μ_ψ is to allow us to extend the functional calculus to $\mathscr{B}(\mathbb{R})$, the bounded Borel functions on $\mathbb{R}$. Let $g \in \mathscr{B}(\mathbb{R})$. It is natural to define $g(A)$ so that $(\psi, g(A)\psi) = \int_{\sigma(A)} g(\lambda)\, d\mu_\psi(\lambda)$. The polarization identity lets us recover $(\psi, g(A)\phi)$ from the proposed $(\psi, g(A)\psi)$ and then the Riesz lemma lets us construct $g(A)$. The properties of this "measurable functional calculus" are given in (Problem 13):

Theorem VII.2 (spectral theorem—functional calculus form) Let A be a bounded self-adjoint operator on $\mathscr{H}$. There is a unique map $\hat{\phi}: \mathscr{B}(\mathbb{R}) \to \mathscr{L}(\mathscr{H})$ so that

(a) $\hat{\phi}$ is an algebraic $*$-homomorphism.
(b) $\hat{\phi}$ is norm continuous: $\|\hat{\phi}(f)\|_{\mathscr{L}(\mathscr{H})} \leq \|f\|_\infty$.
(c) Let f be the function $f(x) = x$; then $\hat{\phi}(f) = A$.
(d) Suppose $f_n(x) \to f(x)$ for each x and $\|f_n\|_\infty$ is bounded. Then $\hat{\phi}(f_n) \to \hat{\phi}(f)$ *strongly*.

Moreover $\hat{\phi}$ has the properties:

(e) If $A\psi = \lambda\psi$, then $\hat{\phi}(f)\psi = f(\lambda)\psi$.
(f) If $f \geq 0$, then $\hat{\phi}(f) \geq 0$.
(g) If $BA = AB$, then $\hat{\phi}(f)B = B\hat{\phi}(f)$.

Theorem VII.2 can be proven directly by extending Theorem VII.1; part (d) requires the dominated convergence theorem. Or, Theorem VII.2 can be proven by an easy corollary of Theorem VII.3 below. The proof of Theorem VII.3 uses only the *continuous* functional calculus. $\hat{\phi}$ extends ϕ and as before we write $\hat{\phi}(f) = f(A)$. As in the continuous functional calculus, one has $f(A)g(A) = g(A)f(A)$.

Since $\mathscr{B}(\mathbb{R})$ is the smallest family closed under limits of form (d) containing all of $C(\mathbb{R})$, we know that any $\hat{\phi}(f)$ is in the smallest C^*-algebra containing A which is also strongly closed; such an algebra is called a von Neumann or W*-algebra. When we study von Neumann algebras in Chapter XVIII we will see that this follows from (g).

The norm equality of Theorem VII.1 carries over if we define $\|f\|'_\infty$ to be the L^∞-norm with respect to a suitable notion of "almost everywhere." Namely, pick an orthonormal basis $\{\psi_n\}$ and say that a property is true a.e. if it is true a.e. with respect to *each* μ_{ψ_i}. Then $\|\hat{\phi}(f)\|_{\mathscr{L}(\mathscr{H})} = \|f\|'_\infty$.

In the next section, we will return to the operators $\chi_\Omega(A)$ where χ_Ω is a characteristic function; this is the most important set of operators in the

measurable but not in the continuous functional calculus. For the time being, we turn to using the spectral measures to form L^2 spaces. We first define:

Definition A vector $\psi \in \mathscr{H}$ is called a **cyclic vector** for A if finite linear combinations of the elements $\{A^n\psi\}_{n=0}^{\infty}$ are dense in $\mathscr{H}$.

Not all operators have cyclic vectors (Problem 14), but if they do:

Lemma 1 Let A be a bounded self-adjoint operator with cyclic vector ψ. Then, there is a unitary operator $U: \mathscr{H} \to L^2(\sigma(A), d\mu_\psi)$ with

$$(UAU^{-1}f)(\lambda) = \lambda f(\lambda)$$

Equality is in the sense of elements of $L^2(\sigma(A), d\mu_\psi)$.

Proof Define U by $U\phi(f)\psi \equiv f$ where f is continuous. U is essentially the inverse of the map ϕ of Theorem VII.1. To show that U is well defined we compute

$$\begin{aligned}\|\phi(f)\psi\|^2 &= (\psi, \phi^*(f)\phi(f)\psi) = (\psi, \phi(\bar{f}f)\psi)\\ &= \int |f(\lambda)|^2 \, d\mu_\psi\end{aligned}$$

Therefore, if $f = g$ a.e. with respect to μ_ψ, then $\phi(f)\psi = \phi(g)\psi$. Thus U is well defined on $\{\phi(f)\psi \mid f \in C(\sigma(A))\}$ and is norm preserving. Since ψ is cyclic $\overline{\{\phi(f)\psi \mid f \in C(\sigma(A))\}} = \mathscr{H}$, so by the B.L.T. theorem U extends to an isometric map of $\mathscr{H}$ into $L^2(\sigma(A), d\mu_\psi)$. Since $C(\sigma(A))$ is dense in L^2, Ran $U = L^2(\sigma(A), d\mu_\psi)$. Finally, if $f \in C(\sigma(A))$,

$$\begin{aligned}(UAU^{-1}f)(\lambda) &= [UA\phi(f)](\lambda)\\ &= [U\phi(xf)](\lambda)\\ &= \lambda f(\lambda)\end{aligned}$$

By continuity, this extends from $f \in C(\sigma(A))$ to $f \in L^2$. ∎

To extend this lemma to arbitrary A, we need to know that A has a family of invariant subspaces spanning $\mathscr{H}$ so that A is cyclic on each subspace:

Lemma 2 Let A be a self-adjoint operator on a separable Hilbert space $\mathscr{H}$. Then there is a direct sum decomposition $\mathscr{H} = \bigoplus_{n=1}^{N} \mathscr{H}_n$ with $N = 1, 2, \ldots,$ *or* ∞ so that:

(a) A leaves each $\mathscr{H}_n$ **invariant**, that is, $\psi \in \mathscr{H}_n$ implies $A\psi \in \mathscr{H}_n$.

(b) For each n, there is a $\phi_n \in \mathscr{H}_n$ which is cyclic for $A \restriction \mathscr{H}_n$, i.e. $\mathscr{H}_n = \overline{\{f(A)\phi_n \mid f \in C(\sigma(A))\}}$.

Proof A simple Zornication (Problem 15).

We can now combine Lemmas 1 and 2 to prove the form of the spectral theorem which we regard as the most transparent:

Theorem VII.3 (spectral theorem—multiplication operator form) Let A be a bounded self-adjoint operator on $\mathscr{H}$, a separable Hilbert space. Then, there exist measures $\{\mu_n\}_{n=1}^N$ ($N = 1, 2, \ldots$ or ∞) on $\sigma(A)$ and a unitary operator

$$U: \mathscr{H} \to \bigoplus_{n=1}^{N} L^2(\mathbb{R}, d\mu_n)$$

so that

$$(UAU^{-1}\psi)_n(\lambda) = \lambda\psi_n(\lambda)$$

where we write an element $\psi \in \bigoplus_{n=1}^N L^2(\mathbb{R}, d\mu_n)$ as an N-tuple $\langle\psi_1(\lambda), \ldots, \psi_N(\lambda)\rangle$. This realization of A is called a **spectral representation.**

Proof Use Lemma 2 to find the decomposition and then use Lemma 1 on each component. ∎

This theorem tells us that every bounded self-adjoint operator is a multiplication operator on a suitable measure space; what changes as the operator changes are the underlying measures. Explicitly:

Corollary Let A be a bounded self-adjoint operator on a separable Hilbert space $\mathscr{H}$. Then there exists a *finite* measure space $\langle M, \mu\rangle$, a bounded function F on M, and a unitary map, $U: \mathscr{H} \to L^2(M, d\mu)$, so that

$$(UAU^{-1}f)(m) = F(m)f(m)$$

Proof Choose the cyclic vectors ϕ_n so that $\|\phi_n\| = 2^{-n}$. Let $M = \bigcup_{n=1}^N \mathbb{R}$, i.e. the union of N copies of $\mathbb{R}$. Define μ by requiring that its restriction to the nth copy of $\mathbb{R}$ be μ_n. Since $\mu(M) = \sum_{n=1}^N \mu_n(\mathbb{R}) < \infty$, μ is finite. ∎

We also notice that this last theorem is essentially a rigorous form of the physicists' Dirac notation. If we write $\psi_n(x) = \psi(x; n)$, we see that in the "new representation defined by U" one has

$$(\psi, \phi) = \sum_n \int d\mu_n \overline{\psi(\lambda; n)}\phi(\lambda; n)$$

$$(\psi, A\phi) = \sum_n \int d\mu_n \overline{\psi(\lambda; n)}\lambda\phi(\lambda; n)$$

These are the Dirac type formulas familiar to physicists except that the formal sums of Dirac are replaced with integrals over spectral measures, where we define:

Definition The measures $d\mu_n$ are called **spectral measures**; they are just $d\mu_\psi$ for suitable ψ.

These measures are *not* uniquely determined and we will eventually discuss this nonuniqueness question. First, let us consider a few examples:

Example 1 Let A be an $n \times n$ self-adjoint matrix. The "usual" finite-dimensional spectral theorem says that A has a complete orthonormal set of eigenvectors, $\psi_1, \ldots, \psi_n$, with $A\psi_i = \lambda_i \psi_i$. Suppose first that the eigenvalues are distinct. Consider the sum of Dirac measures, $\mu = \sum_{i=1}^n \delta(x - \lambda_i)$. $L^2(\mathbb{R}, d\mu)$ is just $\mathbb{C}^n$ since $f \in L^2$ is determined by $f = \langle f(\lambda_1), \ldots, f(\lambda_n)\rangle$. Clearly, the function λf corresponds to the n-tuple $\langle \lambda_1 f(\lambda_1), \ldots, \lambda_n f(\lambda_n)\rangle$, so A is multiplication by λ on $L^2(\mathbb{R}, d\mu)$. If we take $\tilde{\mu} = \sum_{i=1}^n a_i \delta(x - \lambda_i)$ with $a_1, \ldots, a_n > 0$, A can also be represented as multiplication by λ on $L^2(\mathbb{R}, d\tilde{\mu})$. Thus, we explicitly see the nonuniqueness of the measure in this case. We can also see when more than one measure is needed: one can represent a finite-dimensional self-adjoint operator as multiplication on $L^2(\mathbb{R}, d\mu)$ with only one measure if and only if A has no repeated eigenvalues.

Example 2 Let A be compact and self-adjoint. The Hilbert–Schmidt theorem tells us there is a complete orthonormal set of eigenvectors $\{\psi_n\}_{n=1}^\infty$ with $A\psi_n = \lambda_n \psi_n$. If there is no repeated eigenvalue, $\sum_{n=1}^\infty 2^{-n}\delta(x - \lambda_n)$ works as a spectral measure.

Example 3 Let $\mathscr{H} = \ell^2(-\infty, \infty)$, that is, the set of sequences, $\{a_n\}_{n=-\infty}^\infty$ with $\sum_{n=-\infty}^\infty |a_n|^2 < \infty$. Let $L\colon \mathscr{H} \to \mathscr{H}$ by $(La)_n = a_{n+1}$, that is, L shifts to the left. $L^* = R$ with $(Ra)_n = a_{n-1}$. Let $A = R + L$ which is self-adjoint. Can we represent A as a multiplication operator? Map $\mathscr{H}$ into $L^2[0, 1]$ by $U\colon \{a_n\} \to \sum_{n=-\infty}^\infty a_n e^{2\pi i n x}$. Then ULU^{-1} is multiplication by $e^{-2\pi i x}$ and URU^{-1} is multiplication by $e^{+2\pi i x}$ so UAU^{-1} is multiplication by $2\cos(2\pi x)$. The necessary transformations needed to represent A as multiplication by x on $L^2(\mathbb{R}, d\mu_1) \oplus L^2(\mathbb{R}, d\mu_2)$ are left for the problems. μ_1 and μ_2 have support in $[-2, 2]$.

Example 4 Consider $i^{-1}d/dx$ on $L^2(\mathbb{R}, dx)$. This is an unbounded operator and thus not strictly within the context of this section, but we will prove an analogue of Theorem VII.3 in Section VIII.3. We thus seek an operator U and a measure $d\mu$ (it turns out that only one μ is needed) with U: $L^2(\mathbb{R}, dx) \to L^2(\mathbb{R}, d\mu(k))$ so that

$$U\left(\frac{1}{i}\frac{d}{dx}f\right)(k) = kUf(k)$$

The Fourier transform $(Uf)(k) = (2\pi)^{-1/2}\int f(x)e^{-ikx}\,dx$ which we study in Chapter IX precisely does the trick. Thus, the Fourier transform is one example of a spectral representation.

We now investigate the connection between spectral measures and the spectrum.

Definition If $\{\mu_n\}_{n=1}^N$ is a family of measures, the **support** of $\{\mu_n\}$ is the complement of the largest open set B with $\mu_n(B) = 0$ for all n; so

$$\operatorname{supp}\{\mu_n\} = \overline{\bigcup_{n=1}^{N} \operatorname{supp}\mu_n}$$

Proposition Let A be a self-adjoint operator and $\{\mu_n\}_{n=1}^N$ a family of spectral measures. Then

$$\sigma(A) = \operatorname{supp}\{\mu_n\}_{n=1}^N$$

There is also a simple description of $\sigma(A)$ in terms of the more general multiplication operators discussed after Theorem VII.3:

Definition Let F be a real-valued function on a measure space $\langle M, \mu\rangle$. We say λ is in the **essential range** of F if and only if

$$\mu\{m \mid \lambda - \varepsilon < F(m) < \lambda + \varepsilon\} > 0$$

for all $\varepsilon > 0$.

Proposition Let F be a bounded real-valued function on a measure space $\langle M, \mu\rangle$. Let T_F be the operator on $L^2(M, d\mu)$ given by

$$(T_F g)(m) = F(m)g(m)$$

Then $\sigma(T_F)$ is the essential range of F.

Proof See Problem 17b.

We can now see exactly what information is contained in the spectrum. A unitary invariant of a self-adjoint operator A is a property P so that $P(A) = P(UAU^{-1})$ for all unitary operators U. Thus, unitary invariants are "intrinsic" properties of self-adjoint operators, that is, properties independent of "representation." An example of such a **unitary invariant** is the spectrum $\sigma(A)$. However, the spectrum is a poor invariant: for example, multiplication by x on $L^2([0, 1], dx)$ and an operator with a complete set of eigenfunctions having all rationals in $[0, 1]$ as eigenvalues are very different even though both have spectrum $[0, 1]$.

At the conclusion of this section, we will see that there is a canonical choice of "spectral measures" which forms a complete set of unitary invariants, that is, a set of properties which distinguish two self-adjoint operators A and B unless $A = UBU^{-1}$ for some unitary operator U. This explains why $\sigma(A)$ is such a bad invariant for different sorts of measures can have the same support. If we wish to find better invariants which are, however, simpler than measures, it is reasonable to first decompose spectral measures in some natural way and then pass to supports. Recall Theorem I.13 which says that any measure μ on $\mathbb{R}$ has a unique decomposition into $\mu = \mu_{pp} + \mu_{ac} + \mu_{sing}$ where μ_{pp} is a pure point measure, μ_{ac} is absolutely continuous with respect to Lebesgue measure, and μ_{sing} is continuous and singular with respect to Lebesgue measure. These three pieces are mutually singular so

$$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{pp}) \oplus L^2(\mathbb{R}, d\mu_{ac}) \oplus L^2(\mathbb{R}, d\mu_{sing})$$

It is easy to see (Problem 18) that any $\psi \in L^2(\mathbb{R}, d\mu)$ has an absolutely continuous spectral measure $d\mu_\psi$ if and only if $\psi \in L^2(\mathbb{R}, d\mu_{ac})$, and similarly for pure point and singular measures. If $\{\mu_n\}_{n=1}^N$ is a family of spectral measures, we can sum $\bigoplus_{n=1}^N L^2(\mathbb{R}, d\mu_{n;ac})$ by defining:

Definition Let A be a bounded self-adjoint operator on $\mathscr{H}$. Let $\mathscr{H}_{pp} = \{\psi \mid \mu_\psi \text{ is pure point}\}$, $\mathscr{H}_{ac} = \{\psi \mid \mu_\psi \text{ is absolutely continuous}\}$, $\mathscr{H}_{sing} = \{\psi \mid \mu_\psi \text{ is continuous singular}\}$.

We have thus proven:

Theorem VII.4 $\mathscr{H} = \mathscr{H}_{pp} \oplus \mathscr{H}_{ac} \oplus \mathscr{H}_{sing}$. Each of these subspaces is invariant under A. $A \restriction \mathscr{H}_{pp}$ has a complete set of eigenvectors, $A \restriction \mathscr{H}_{ac}$ has only absolutely continuous spectral measures and $A \restriction \mathscr{H}_{sing}$ has only continuous singular spectral measures.

Definition
$$\sigma_{pp}(A) = \{\lambda \mid \lambda \text{ is an eigenvalue of } A\}$$
$$\sigma_{cont}(A) = \sigma(A \restriction \mathscr{H}_{cont} \equiv \mathscr{H}_{sing} \oplus \mathscr{H}_{ac})$$
$$\sigma_{ac}(A) = \sigma(A \restriction \mathscr{H}_{ac})$$
$$\sigma_{sing}(A) = \sigma(A \restriction \mathscr{H}_{sing})$$

These sets are called the **pure point, continuous, absolutely continuous,** and **singular** (or **continuous singular) spectrum** respectively.

While it may happen that $\sigma_{ac} \bigcup \sigma_{sing} \bigcup \sigma_{pp} \neq \sigma$, this is only true because we did not define σ_{pp} as $\sigma(A \restriction \mathscr{H}_{pp})$ but rather as the actual set of eigenvalues. One always has

Proposition
$$\sigma_{cont}(A) = \sigma_{ac}(A) \bigcup \sigma_{sing}(A)$$
$$\sigma(A) = \overline{\sigma_{pp}(A)} \bigcup \sigma_{cont}(A)$$

The sets need not be disjoint, however. The reader should be warned that $\sigma_{sing}(A)$ may have nonzero Lebesgue measure (Problem 7). For many purposes, breaking up the spectrum in this way gives useful information. In Section VII.3, we introduce another breakup which is also useful.

As we discussed in the notes to Section VI.3, some authors use a notion of "continuous spectrum" which is distinct from the above, namely they define the continuous spectrum to be the set of $\lambda \in \sigma(T)$ which are neither in the point spectrum nor in the residual spectrum. To illustrate the difference between the two definitions we let $\mathscr{H} = \mathbb{C} \oplus L^2[0, 1]$ and define A: $\langle \alpha, f(x) \rangle \to \langle \frac{1}{2}\alpha, xf(x) \rangle$. With our definition, the point $\lambda = \frac{1}{2}$ is in both the pure point and the continuous spectrum. The other authors assign $\lambda = \frac{1}{2}$ to the point spectrum and their continuous spectrum is $[0, \frac{1}{2}) \cup (\frac{1}{2}, 1]$.

Finally, we turn to the question of making canonical choices for the spectral measures, a subject which goes under the title of "multiplicity theory." We will describe the basic results without proof:

1. Multiplicity free operators

We must first ask when A is unitarily equivalent to multiplication by x on $L^2(\mathbb{R}, d\mu)$, that is, when only one spectral measure is needed. A look at Example 1 tells us this happens in the finite-dimensional case only when A has no repeated eigenvalues, so we define:

Definition A bounded self-adjoint operator A is called **multiplicity free** if and only if A is unitarily equivalent to multiplication by λ on $L^2(\mathbb{R}, d\mu)$ for some measure μ.

One is interested in intrinsic characterizations of "multiplicity free" and there are several:

Theorem VII.5 The following are equivalent:

(a) A is multiplicity free.
(b) A has a cyclic vector.
(c) $\{B \mid AB = BA\}$ is an abelian algebra.

2. Measure classes

Next we must ask about the nonuniqueness of the measure in the multiplicity free case. The situation in the finite-dimensional multiplicity free case was seen in Example 1: the "acceptable" measures were $\sum_{n=1}^{N} \alpha_n \delta(\lambda - \lambda_n)$ with each $\alpha_n \neq 0$. There is a natural generalization. Suppose $d\mu$ on $\mathbb{R}$ is given and let F be a measurable function which is positive and nonzero a.e. with respect to μ and locally $L^1(\mathbb{R}, d\mu)$, that is, $\int_C |F|\, d\mu < \infty$ for every compact set $C \subset \mathbb{R}$. Then $d\nu = F\, d\mu$ is a Borel measure and the map, U,

$$U: L^2(\mathbb{R}, d\nu) \to L^2(\mathbb{R}, d\mu)$$

given by $(Uf)(\lambda) = \sqrt{F(\lambda)} f(\lambda)$ is unitary (onto since $F \neq 0$ a.e.) and $\lambda(Uf) = U(\lambda f)$. Thus, an operator A with a spectral representation in terms of μ could just as well be represented in terms of ν. By the Radon–Nikodym theorem, $d\nu = F\, d\mu$ with F a.e. nonzero if and only if ν and μ have the same sets of measure zero. This suggests the definition:

Definition Two Borel measures μ and ν are called **equivalent** if and only if they have the same sets of measure zero. An equivalence class $\langle \mu \rangle$ is called a **measure class.**

Then, the nonuniqueness question is answered by:

Proposition Let μ and ν be Borel measures on $\mathbb{R}$ with bounded support. Let A_μ be the operator on $L^2(\mathbb{R}, d\mu)$ given by $(A_\mu f)(\lambda) = \lambda f(\lambda)$ and similarly for A_ν on $L^2(\mathbb{R}, d\nu)$. Then A_μ and A_ν are unitarily equivalent if and only if μ and ν are equivalent measures.

3. Operators of uniform multiplicity

If one wants a canonical listing of the eigenvalues of a matrix, it is natural to list all eigenvalues of multiplicity one, all eigenvalues of multiplicity two, etc. We thus need a way of saying that A is an operator of uniform multiplicity two, three, etc. It is natural to take:

Definition A bounded self-adjoint operator A is said to be of **uniform multiplicity** m if A is unitarily equivalent to multiplication by λ on $L^2(\mathbb{R}, d\mu) \oplus \cdots \oplus L^2(\mathbb{R}, d\mu)$ where there are m terms in the sum and μ is a fixed Borel measure.

That this is a good definition is shown by

Proposition If A is unitarily equivalent to multiplication by λ on $L^2(\mathbb{R}, d\mu) \oplus \cdots \oplus L^2(\mathbb{R}, d\mu)$ (m times) and on $L^2(\mathbb{R}, d\nu) \oplus \cdots \oplus L^2(\mathbb{R}, d\nu)$ (n times), then $m = n$ and μ and ν are equivalent measures.

4. Disjoint measure classes

In listing eigenvalues of multiplicity one, two, three, etc. in the finite-dimensional case, we must add a requirement that prevents us from counting an eigenvalue of multiplicity three once as an eigenvalue of multiplicity one and once as an eigenvalue of multiplicity two. In the finite-dimensional case, we avoid this "error" by requiring the lists to be disjoint. The analogous notion for measures is:

Definition Two measure classes $\langle \mu \rangle$ and $\langle \nu \rangle$ are called **disjoint** if any $\mu_1 \in \langle \mu \rangle$ and $\nu_1 \in \langle \nu \rangle$ are mutually singular.

5. The multiplicity theorem

We can now state the basic theorem:

Theorem VII. 6 (commutative multiplicity theorem) Let A be a bounded self-adjoint operator on a Hilbert space $\mathscr{H}$. Then there is a decomposition $\mathscr{H} = \mathscr{H}_1 \oplus \mathscr{H}_2 \oplus \cdots \oplus \mathscr{H}_\infty$ so that

(a) A leaves each $\mathscr{H}_m$ invariant.
(b) $A \restriction \mathscr{H}_m$ has uniform multiplicity m.

(c) The measure classes $\langle \mu_m \rangle$ associated with the spectral representation of $A \restriction \mathscr{H}_m$ are mutually disjoint.

Moreover, the subspaces $\mathscr{H}_1, \ldots, \mathscr{H}_m, \ldots, \mathscr{H}_\infty$ (some of which may be zero) and the *measure classes* $\langle \mu_1 \rangle, \ldots, \langle \mu_m \rangle, \ldots, \langle \mu_\infty \rangle$ are uniquely determined by (a)–(c).

The spectral theorem with the multiplicity theory just described is thus one of those gems of mathematics: a structure theorem, that is, a theorem that describes all objects of a certain sort up to a natural equivalence. Each bounded self-adjoint operator A is described by a family of mutually disjoint measure classes on $[-\|A\|, \|A\|]$; two operators are unitarily equivalent if and only if their spectral multiplicity measure classes are *identical.*

VII.3 Spectral projections

In the last section, we constructed a functional calculus, $f \mapsto f(A)$ for any Borel function f and any bounded self-adjoint operator A. The most important functions gained in passing from the continuous functional calculus to the Borel functional calculus are the characteristic functions of sets.

Definition Let A be a bounded self-adjoint operator and Ω a Borel set of $\mathbb{R}$. $P_\Omega \equiv \chi_\Omega(A)$ is called a **spectral projection** of A.

As the definition suggests, P_Ω is an orthogonal projection since $\chi_\Omega^2 = \chi_\Omega = \bar{\chi}_\Omega$ pointwise. The properties of the family of projections $\{P_\Omega \mid \Omega$ an arbitrary Borel set$\}$ is given by the following elementary translation of the functional calculus (Problem 22).

Proposition The family $\{P_\Omega\}$ of spectral projections of a bounded self-adjoint operator, A, has the following properties:

(a) Each P_Ω is an orthogonal projection.
(b) $P_\varnothing = 0$; $P_{(-a,a)} = I$ for some a.
(c) If $\Omega = \bigcup_{n=1}^\infty \Omega_n$ with $\Omega_n \cap \Omega_m = \varnothing$ for all $n \neq m$, then

$$P_\Omega = \operatorname*{s-lim}_{N \to \infty} \left(\sum_{n=1}^{N} P_{\Omega_n} \right)$$

(d) $P_{\Omega_1} P_{\Omega_2} = P_{\Omega_1 \cap \Omega_2}$

Condition (c) is very reminiscent of the condition defining a measure and in fact one defines:

Definition A family of projections obeying (a)–(c) is called a (bounded) **projection-valued measure** (p.v.m.).

We remark that (d) follows from (a) and (c) by abstract considerations (Problem 22).

As one might guess, one can integrate with respect to a p.v.m. If P_Ω is a p.v.m., then $(\phi, P_\Omega \phi)$ is an ordinary measure for any ϕ. We will use the symbol $d(\phi, P_\lambda \phi)$ to mean integration with respect to this measure. By standard Riesz lemma methods, there is a unique operator B with $(\phi, B\phi) = \int f(\lambda)\, d(\phi, P_\lambda \phi)$. Thus:

Theorem VII.7 If P_Ω is a p.v.m. and f a bounded Borel function on $\operatorname{supp} P_\Omega$, then there is a unique operator B which we denote $\int f(\lambda)\, dP_\lambda$ so that

$$(\phi, B\phi) = \int f(\lambda)\, d(\phi, P_\lambda \phi), \qquad \forall \phi \in \mathscr{H}$$

Example If A is a bounded self-adjoint operator and $\{P_\Omega\}$ its associated p.v.m., it is easy to see (Problem 23) that $f(A) = \int f(\lambda)\, dP_\lambda$. In particular $A = \int \lambda\, dP_\lambda$.

Now, suppose a bounded p.v.m. P_Ω is given and we form $A = \int \lambda\, dP_\lambda$. Not surprisingly (Problem 23), P_Ω is just the p.v.m. associated with A. Summarizing:

Theorem VII.8 (spectral theorem—p.v.m. form) There is a one–one correspondence between (bounded) self-adjoint operators A and (bounded) projection valued measures $\{P_\Omega\}$ given by:

$$A \mapsto \{P_\Omega\} = \{\chi_\Omega(A)\}$$

$$\{P_\Omega\} \mapsto A = \int \lambda\, dP_\lambda$$

It is through this theorem and its generalization to unbounded operators that self-adjoint operators arise in quantum mechanics, for the observables occur most naturally as projection-valued measures (see Section VIII.3 for

the generalization and the notes to Section VIII.11 for the quantum-mechanical explanation).

Spectral projections can be used to investigate the spectrum of A:

Proposition $\lambda \in \sigma(A)$ if and only if $P_{(\lambda-\varepsilon,\,\lambda+\varepsilon)}(A) \neq 0$ for any $\varepsilon > 0$.

The essential element of the proof is that $\|(A-\lambda)^{-1}\| = [\text{dist}(\lambda, \sigma(A))]^{-1}$ The details are left to Problem 24.

This suggests that we distinguish between two types of spectrum:

Definition We say $\lambda \in \sigma_{\text{ess}}(A)$, the **essential spectrum** of A, if and only if $P_{(\lambda-\varepsilon,\,\lambda+\varepsilon)}(A)$ is infinite dimensional for all $\varepsilon > 0$. If $\lambda \in \sigma(A)$, but $P_{(\lambda-\varepsilon,\,\lambda+\varepsilon)}(A)$ is finite dimensional for some $\varepsilon > 0$, we say $\lambda \in \sigma_{\text{disc}}(A)$, the **discrete spectrum** of A. P is infinite dimensional means Ran P is infinite dimensional.

Thus, we have a second decomposition of $\sigma(A)$. Unlike the first, it is a decomposition into two necessarily disjoint subsets. We note that σ_{disc} is not necessarily closed, but:

Theorem VII.9 $\sigma_{\text{ess}}(A)$ is always closed.

Proof Let $\lambda_n \to \lambda$ with each $\lambda_n \in \sigma_{\text{ess}}(A)$. Since any open interval I about λ contains an interval about some λ_n, $P_I(A)$ is infinite dimensional. ∎

The following three theorems give alternative descriptions of σ_{disc} and σ_{ess}; their proofs are left to the reader (Problem 26).

Theorem VII.10 $\lambda \in \sigma_{\text{disc}}$ if and only if *both* the following hold:

(a) λ is an isolated point of $\sigma(A)$, that is, for some ε, $(\lambda-\varepsilon, \lambda+\varepsilon) \cap \sigma(A) = \{\lambda\}$.

(b) λ is an eigenvalue of finite multiplicity, i.e., $\{\psi \mid A\psi = \lambda\psi\}$ is finite dimensional.

Theorem VII.11 $\lambda \in \sigma_{\text{ess}}$ if and only if *one* or more of the following holds:

(a) $\lambda \in \sigma_{\text{cont}}(A) \equiv \sigma_{\text{ac}}(A) \cup \sigma_{\text{sing}}(A)$.

(b) λ is a limit point of $\sigma_{\text{pp}}(A)$.

(c) λ is an eigenvalue of infinite multiplicity.

Theorem VII.12 (Weyl's criterion) Let A be a bounded self-adjoint operator. Then $\lambda \in \sigma(A)$ if and only if there exists $\{\psi_n\}_{n=1}^{\infty}$ so that $\|\psi_n\| = 1$ and $\lim_{n\to\infty} \|(A - \lambda)\psi_n\| = 0$. $\lambda \in \sigma_{ess}(A)$ if and only if the above $\{\psi_n\}$ can be chosen to be orthogonal.

As one might guess, the essential spectrum cannot be removed by essentially finite dimensional perturbations. In Section XIII.4, we will prove a general theorem which implies that $\sigma_{ess}(A) = \sigma_{ess}(B)$ if $A - B$ is compact.

Finally, we discuss one useful formula relating the resolvent and spectral projections. It is a matter of computation to see that

$$f_\varepsilon(x) \to \begin{cases} 0 & x \notin [a, b] \\ \frac{1}{2} & x = a \text{ or } x = b \\ 1 & x \in (a, b) \end{cases}$$

if $\varepsilon \downarrow 0$ where

$$f_\varepsilon(x) = \frac{1}{2\pi i} \int_a^b \left(\frac{1}{x - \lambda - i\varepsilon} - \frac{1}{x - \lambda + i\varepsilon} \right) d\lambda$$

Moreover, $|f_\varepsilon(x)|$ is bounded uniformly in ε, so by the functional calculus, one has:

Theorem VII.13 (Stone's formula) Let A be a bounded self-adjoint operator. Then

$$\text{s-}\lim_{\varepsilon\downarrow 0} (2\pi i)^{-1} \int_a^b [(A - \lambda - i\varepsilon)^{-1} - (A - \lambda + i\varepsilon)^{-1}]\, d\lambda = \tfrac{1}{2}[P_{[a,b]} + P_{(a,b)}]$$

VII.4 Ergodic theory revisited: Koopmanism

In Section II.4 we defined ergodicity for a measure preserving bijective map, $T: \Omega \to \Omega$ where Ω is a measure space with a finite measure μ, and $\mu(T^{-1}(M)) = \mu(M)$ for any measurable set $M \subset \Omega$. Koopman's lemma told us that the map U defined by $(Uf)(w) = f(Tw)$, is a unitary operator on $L^2(\Omega, d\mu)$. T was called ergodic if and only if 1 was a simple eigenvalue of U (that is, an eigenvalue of multiplicity one). In this section, we wish to examine in detail the idea of Koopman that interesting properties of T can be described in terms of spectral properties of U.

To appreciate the notion of mixing which we will shortly introduce, let us first consider an example:

Example 1 Let Ω be the surface of a torus: We can think of Ω as all pairs of numbers $\langle x, y\rangle$ with $0 \le x < 1$; $0 \le y < 1$ topologized so neighborhoods of 0 include points near 1. We consider two pairs $\langle x, y\rangle$ and $\langle z, w\rangle$ of reals as equivalent if $x - z$ and $y - w$ are integral. Then Ω is also all equivalence classes of pairs. Let us define a two-parameter family of maps $T_{a,b}$: $\Omega \to \Omega$ by $T_{a,b}\langle x, y\rangle = \langle x + a, y + b\rangle$. $T_{a,b}$ is Lebesgue measure preserving. When is $T_{a,b}$ ergodic relative to Lebesgue measure? If one uses the definition of ergodic which requires that there be no invariant sets of measure different from 1 or 0, it is not clear which $T_{a,b}$ are ergodic. However, if one looks at $(U_{a,b}f)(x, y) = f(x + a, y + b)$, one notices that it has a complete family of eigenvectors, $\varphi_{n,m}(x, y) = \exp[2\pi i(nx + my)]$. $U_{a,b}\varphi_{n,m} = \exp[2\pi i(na + mb)] \times \varphi_{n,m}$. When is 1 a simple eigenvalue? Obviously, if and only if $na + mb = k$ has no solution with n, m and k integral, except for $n = m = 0$ (e.g. when $a = \pi, b = \sqrt{2}$).

Thus $T_{\pi,\sqrt{2}}$ is ergodic, so space averages equal time averages in this case. This happens because the images $\{T^n w \mid w \in \Omega\}$ are a set which is dense and fairly uniform rather than because T^n takes a small neighborhood of w and

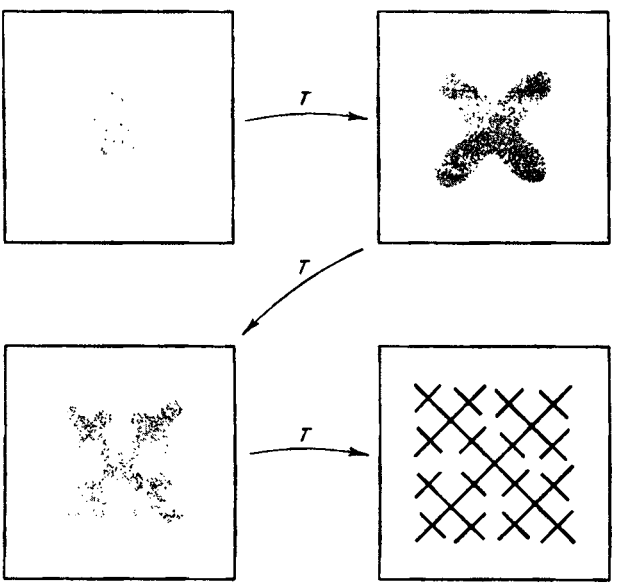

FIGURE VII.1 The intuitive idea of thermodynamic behavior in phase space.

spreads it all out as in Figure VII.1. In fact T^n is "shape preserving in this case." We expect "irreversibility" to mean that nearby points w and u are not nearby after many iterates of T.

How can we describe what it means to have a set M spread out "uniformly" upon iteration? One should expect a point to "forget" at what time it started in A, that is, the probability of being in T^nA and another set B should approach an n-independent limit.

Definition A measure preserving transformation $T: \Omega \to \Omega$ on a measure space $\langle \Omega, \mu \rangle$ with $\mu(\Omega) = 1$ is called **mixing** if and only if for all measurable sets A and B in Ω:

$$\lim_{n\to\infty} \mu(T^nA \cap B) = \mu(A)\mu(B)$$

If T is ergodic, then by the mean ergodic theorem:

$$\begin{aligned}\lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} \mu(T^mA \cap B) &= \lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} (U^{-m}\chi_A, \chi_B) \\ &= (\chi_A, 1)(1, \chi_B) \\ &= \mu(A)\mu(B)\end{aligned}$$

Thus, ergodicity is equivalent to the mixing limit existing in a Cesaro sense, so that mixing implies ergodicity. Alternatively, we can see this directly. If $T[A] = A$, then $\lim_{n\to\infty} \mu(T^nA \cap A) = \mu(A)$ so mixing implies that $\mu(A)^2 = \mu(A)$, i.e. $\mu(A) = 0$ or 1. Before stating that mixing implies ergodicity as a formal proposition we introduce an intermediate notion:

Definition A measure preserving transformation $T: \Omega \to \Omega$ on a measure space $\langle \Omega, \mu \rangle$ with $\mu(\Omega) = 1$ is called **weakly mixing** if and only if for all measurable sets A and B in Ω:

$$\lim_{n\to\infty} \frac{1}{n} \sum_{m=0}^{n-1} |\mu(T^mA \cap B) - \mu(A)\mu(B)| = 0$$

Clearly:

Proposition Mixing $\Rightarrow$ weakly mixing $\Rightarrow$ ergodicity.

Let us first consider an example which we will shortly prove is mixing. We will see that Example 1 is *not* mixing.

and $x_n = 0$, let $\chi_n(x, y) = 1$ and if $x_n = 1$, let $\chi_n(x, y) = -1$. If $n \leq 0$ and $y_{-n+1} = 0$, let $\chi_n(x, y) = 1$ and if $y_{-n+1} = 1$, let $\chi_n(x, y) = -1$. If $\{n_1, \ldots, n_m\}$ is a finite set of integers, define

$$\chi_{\{n_1, \ldots, n_m\}}(x, y) = \prod_{k=1}^{m} \chi_{n_k}(x, y)$$

Define $\chi_\varnothing = 1$. Then:

(a) $\chi_A \chi_B = \chi_{A \Delta B}$ where $A \Delta B = (A \backslash B) \cup (B \backslash A)$

(b) $\int \chi_A \, dx \, dy = \begin{cases} 0 & \text{if } A \neq \varnothing \\ 1 & \text{if } A = \varnothing \end{cases}$

(c) The χ_A are an orthonormal set, by (a) and (b).

(d) If m, n, k and j are integers with $0 < m \leq 2^n$, $0 < k \leq 2^j$, then the characteristic function of

$$\left(\frac{m-1}{2^j}, \frac{m}{2^j}\right] \times \left(\frac{k-1}{2^j}, \frac{k}{2^j}\right]$$

can be written as a finite product $\prod_{m=1}^{N} (1 \pm \chi_{n_m})$ for suitable integers, $n_1, \ldots, n_m$.

(e) The χ_A are an orthonormal basis for $L^2(\Omega, dx \otimes dy)$ for the linear combinations of the characteristic functions of (d) are dense.

(f) $U\chi_{\{n_1, \ldots, n_m\}} = \chi_{\{n_1+1, \ldots, n_m+1\}}$. Thus $\{1\}^\perp$ has an orthonormal basis $\psi_{n,m}$ with $U\psi_{n,m} = \psi_{n+1,m}$. m runs through a countably infinite sequence.

Thus the map in Example 2 is mixing.

Ergodicity, mixing and spectral notions are important not only in statistical mechanical contexts but also in studying the following problem: Let $\langle M, \mu \rangle$ and $\langle N, \nu \rangle$ be measure spaces and let $T: M \to M$ and $S: N \to N$ be measurable transformations which are invertible and measure preserving. When are they equivalent? That is, when is there a $R: M \to N$ so that $T = R^{-1}SR$? R is required to be bijective almost everywhere (i.e. $\mu\{x \mid Ry = Rx \text{ for some } y \neq x\} = 0$ and $\mu\{N \backslash \text{Ran } R\} = 0$) and measure preserving. This is analogous to the unitary equivalence problem for self-adjoint operators which is solved by the multiplicity theorems, but it has *not* been completely solved. In Problem 29 we construct various maps equivalent to the Baker's transformation.

The unitary equivalence problem for self-adjoint operators was solved by finding a *complete* set of invariants. Koopmanism immediately gives a whole family of invariants of measure preserving maps, for if $T: M \to M$ and $S: N \to N$ are equivalent, the induced unitaries are unitarily equivalent. Given a measure preserving transformation, T, the multiplicity measure classes of the associated unitary operator are invariants for T, i.e. if S and T

are related by $T = R^{-1}SR$, then their classes are the same. Since ergodicity and mixing are expressible in terms of the induced Koopman unitaries they are not additional invariants. Are these invariants associated with the induced unitaries complete? That is, if the induced unitaries are unitarily equivalent, is it necessarily true that there exists an R so that $T = R^{-1}SR$? Under some special additional assumptions, the answer is yes.

Theorem VII.16 (Halmos, von Neumann) Let $T: M \to M$ and $S: N \to N$ be measure-preserving ergodic transformations, U_S and V_T the induced unitaries. Suppose U_S and V_T have only pure point spectrum. Then T and S are measure theoretically equivalent if and only if U_S and V_T are unitarily equivalent.

On the other hand, Kolmogorov and Sinai have constructed an invariant (called the entropy) for a class of mixing measurable transformations called K-systems. On $\{1\}^{\perp}$, the unitary induced by a K-system has an orthonormal basis $\{\psi_{n,m}\}_{n,m=-\infty}^{\infty}$ with $U\psi_{n,m} = \psi_{n+1,m}$. Thus, the unitaries induced by K-systems are all unitarily equivalent to one another. But, there exist K-systems with different entropy so the invariants of the induced unitaries do not distinguish all measure-preserving transformations.

NOTES

Section VII.1 For a proof and discussion of the finite dimensional spectral theorem see P. R. Halmos, *Finite Dimensional Vector Spaces*, Van Nostrand-Reinhold, Princeton New Jersey, 1958.

For a related but slightly different proof of Theorem VII.1, see E. Nelson, *Topics in Dynamics*, Vol. I, Princeton Univ. Press, Princeton, New Jersey, 1969.

The general functional calculus, $A \mapsto f(A)$ for functions f analytic in a neighborhood of $\sigma(A)$ which we alluded to is often called the **Dunford functional calculus** after its appearance in N. Dunford, "Spectral Theory I, Convergence to Projections," *Trans. Amer. Math. Soc.* **54** (1943), 185–217. The basic idea is to pick a contour C in the domain of f with $\sigma(A)$ contained within C. Then one takes $f(A) = (2\pi i)^{-1} \oint_C f(z)(z - A)^{-1}\, dz$. Thus, for example, the resolvent identity $(z - A)^{-1}(w - A)^{-1} = (w - z)^{-1}[(z - A)^{-1} - (w - A)^{-1}]$ implies $(fg)(A) = f(A)g(A)$. For further discussion, see N. Dunford and J. Schwartz, *Linear Operators*, Part I, pp. 556–577, Wiley (Interscience), New York, 1958 (also Problem 1).

Section VII.2 For a summary of the history of the spectral theorem, see the article by E. Hellinger and O. Toeplitz, in *Encyklop. Math. Wiss. IIC* **13** (1928), 1335–1616.

The derivation of the functional calculus form of the spectral theorem is also discussed in

Example 2 (the Baker's transformation) Let Ω be the torus. Let

$$T\langle x, y\rangle = \begin{cases} \langle 2x, \tfrac{1}{2}y\rangle & \text{if } 0 \le x < \tfrac{1}{2} \\ \langle 2x - 1, \tfrac{1}{2} + \tfrac{1}{2}y\rangle & \text{if } \tfrac{1}{2} \le x < 1 \end{cases}$$

(see Figure VII.2). One can explicitly see the sets being "ripped apart" by T and "spread around."

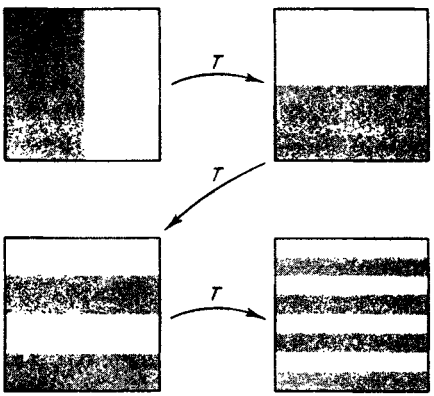

FIGURE VII.2 The Baker's transformation.

Weakly mixing and mixing have simple descriptions in terms of the associated unitary U:

Theorem VII.14 Let T be a measurable transformation and U the associated unitary operator. Then:

(a) U is mixing if and only if

$$w\text{-}\lim_{n\to\infty} U^n = P_1$$

where P_1 is the projection onto the constants, i.e. if and only if

$$\lim_{n\to\infty} (f, U^n g) = (f, 1)(1, g)$$

(b) U is weakly mixing if and only if U has no eigenvalue other than one and one is a simple eigenvalue.

Proof (a) Mixing is clearly implied by $(f, U^n g) \to (f, 1)(1, g)$ for take $f = \chi_A$ and $g = \chi_B$. Conversely, if T is mixing, the limit statement is true if f and g are characteristic functions, and thus also if they are finite linear combinations of characteristic functions. Since these are dense, $\|U^n\| = 1$, and $\|P_1\| = 1$, the result follows.

(b) See references in the Notes. ∎

Example 1 is *not* mixing since $U\psi = \lambda\psi$ implies that $w\text{-lim } U^n\psi \neq P_1\psi$ if $\lambda \neq 1$.

There is a spectral condition on U which often is useful in proving mixing. One can prove a spectral theorem for normal (and thus unitary) operators (Problems 3 and 5) so the notion of absolutely continuous spectrum makes good sense.

Theorem VII.15 Let T be a measure preserving transformation and U the associated unitary operator. Then

(a) If U has purely absolutely continuous spectrum on $\{1\}^\perp$, that is, if $\mathscr{H}_{ac} = \{f \mid (f, 1) = \int f\, d\mu = 0\}$, then T is mixing.

(b) If $\{1\}^\perp$ has an orthonormal basis $\{\varphi_{n,m}\}$, $-\infty < n < \infty$, $1 \leq m < N+1$, where N may be finite or infinite, so that $U\varphi_{n,m} = \varphi_{n+1,m}$, then U has purely absolutely continuous spectrum on $\{1\}^\perp$, and T is mixing.

Proof (a) It is quite easy to see that $U^n \xrightarrow{w} P_1$ if and only if $(f, U^n g) \to 0$ for all $f, g \in \{1\}^\perp$. Suppose that U has purely absolutely continuous spectrum. Then we can find functions $\{F_m\}_{m=1}^N$ and realizations of $f \in \{1\}^\perp$ as $f = \langle f_1(\theta), \ldots, f_m(\theta), \ldots\rangle$ so that

$$(f, U^n g) = \sum_{m=1}^{N} \int_0^{2\pi} e^{in\theta}\overline{f_m(\theta)} g_m(\theta) F_m(\theta)\, d\theta$$

$$= \int_0^{2\pi} e^{in\theta} Q(\theta)\, d\theta$$

where $\int_0^{2\pi} |Q(\theta)|\, d\theta < \infty$. By the Riemann–Lebesgue lemma which we prove in Section IX.2, $(f, U^n g) \to 0$.

(b) On $\{1\}^\perp$, U is just N copies of the right shift on $\ell_2(-\infty, \infty)$. We have analyzed this shift in Example 4 of Section VII.2 and seen that it has absolutely continuous spectrum. ∎

Example 2 *(revisited)* It is intuitively reasonable that the Baker's transformation is mixing and we now have the tools to prove that it is. Let us reexpress T. Write $\langle x, y\rangle \in \Omega$ in a base two decimal expansion $x = .x_1x_2\cdots$; $y = .y_1y_2\cdots$ with each $x_i = 0$ or 1 and each $y_i = 0$ or 1. Then

$$T\colon (.x_1x_2\cdots, .y_1y_2\cdots) \to (.x_2x_3\cdots, .x_1y_1y_2\cdots),$$

i.e. if we write a point in Ω as $(\ldots, y_3, y_2, y_1, x_1, x_2, \ldots)$ T is just a left shift. Warning: this is not the same as saying U is a left shift! This suggests what we should do. Define the functions $\chi_n(x, y)$ on Ω as follows: If $n > 0$

J. Diximier, *Les Algèbres d'Opérateurs dans l'Espace Hilbertien*, Gauthier, Paris, 1957, Appendix. The multiplication operator form is discussed in Nelson (ref. to Section VII.1) pp. 66–74.

There has arisen an extensive literature on a "rigorous" Dirac notation which attempts to capture the flavor of bras and kets more fully. For the original Dirac notation, see P. A. M. Dirac, *The Principles of Quantum Mechanics*, Oxford Univ. Press (Clarendon), London and New York, 1935. For the rigorous forms in terms of "rigged Hilbert spaces" see K. Maurin, *General Eigenfunction Expansions and Unitary Representations of Topological Groups*, Polish Scientific Publ., 1968; J. Roberts," The Dirac Bra and Ket Formalism," *J. Math. Phys.* 7 (1966), 1097–1104; "Rigged Hilbert Spaces in Quantum Mechanics," *Commun. Math. Phys.* **3** (1966), 98–119; or J. P. Antoine, "Dirac Formalism and Symmetry Problems in Quantum Mechanics I, II," *J. Math. Phys.* **10** (1969), 53–69, 2277–2290. We must emphasize that we regard the spectral theorem as sufficient for any argument where a nonrigorous approach might rely on Dirac notation; thus, we only recommend the abstract rigged space approach to readers with a strong emotional attachment to the Dirac formalism.

For an additional discussion of σ_{ac}, σ_{sing}, σ_{pp}, see T. Kato, *Perturbation Theory for Linear Operators*, pp. 516–519, Springer-Verlag, Berlin and New York, 1966.

The multiplicity theory for self-adjoint operators dates back at least as far as: H. Hahn, "Uber die Integrale des Herrn Hellinger und die orthogonalinvarianten der quadratischen Formen von unendlichen Veränderlichen," *Monatsh. Math. Phy.* **23** (1912), 161–224 and E. Hellinger, "Neue Begründung der Theorie quadratischen Formen von unendlichvielen Veranderlichen," *J. Reine Angew. Math.* **136** (1907), 210–271. For a modern readable approach, see Nelson (ref. to VII.1) pp. 77–97. The notion of measure class is often the correct continuous analogue to the notion of subset of a discrete set. This idea has been emphasized especially by G. W. Mackey, see *Group Representations and Applications*, pp. 48–80, Oxford Lectures.

Almost all the spectral theory we discuss has a suitable generalization to the nonseparable case. It is for convenience and brevity that we only discuss the separable case.

Section VII.3 For a discussion of the spectral theorem in p.v.m. form and the related "resolution of the identity form," see M. Naimark, *Normed Rings*, Nordhoff, New York, 1964 or E. Lorch, *Spectral Theory*, Oxford Univ. Press, London and New York. Lorch's method of proof is closely linked to the Dunford functional calculus and Stone's formula. See Kato's book (ref. to Section VII.2) for a related point of view.

Stone's formula goes back at least as far as M. Stone's classic book, *Linear Transformations in Hilbert Space and Their Applications to Analysis*, Amer. Math. Soc., Providence, Rhode Island, 1932.

The term essential spectrum goes back to Weyl's famous analysis of singular differential operators, "Uber gewohnliche Differential-gleichungen mit Singularitaten und die zugehorigen Entwicklungen Willkurlicher Functionen," *Math. Ann.* **68** (1910), 220–269; for example, if $H = -d^2/dx^2 + V$ is in the limit point case at infinity and the operators H_λ are the various extensions of H on $L^2(0, \infty)$ with different boundary conditions, Weyl called $\bigcap \sigma(H_\lambda)$ the essential spectrum, that is, the spectrum independent of boundary conditions. It turns out that $\sigma_{ess}(H_\lambda)$ is the same for each λ and is just the Weyl essential spectrum. For discussion of this phenomenon, see Section XIII.4.

Section VII.4 Koopmanism dates back to the fundamental paper of Koopman (see notes to Section II.4). Much of what we discuss may be found in the review article by Wightman and the books of Avez-Arnold and Halmos (notes to Section II.4). In particular, proofs of Theorems VII.14(b) and VII.16 may be found in Halmos' book.

Mixing was introduced by E. Hopf in his note: "Complete Transitivity and the Ergodic Principle," *Proc. Nat. Acad. Sci.* **18** (1932), 204–209.

The theorem of Halmos and von Neumann (Theorem VII.16) was first proven in J. von Neumann, "Zur Operatoren methode in der Klassichen Mechanik," *Ann. Math.* **33** (1932), 587–642. Simplifications and additions may be found in P. R. Halmos and J. von Neumann, "Operator Methods in Classical Mechanics, II," *Ann. Math.* **43** (1942), 332–350. Halmos and von Neumann also prove that the possible discrete spectra of ergodic transformations are all countable subgroups of the circle.

Entropy for K-systems was introduced in A. N. Kolmogorov, "On the Entropy per Time Unit as a Metric Invariant of Automorphisms," *Dokl. Akad. Nauk.* **124** (1959), 754–755. It generalizes the idea of C. Shannon, "A Mathematical Theory of Communication," *Bell. System Tech. J.* **27** (1948), 379–423, 623–656 and is further discussed in J. Sinai, "Dynamical Systems with Countably Multiple Lebesgue Spectrum, I," *Izv. Akad. Nauk. SSSR Mat.* **25** (1961), 899–924 [*Engl. Transl.: Amer. Math. Soc. Transl.* (2) **39** (1964), 83–110]. For a readable introduction to the theory, see P. Billingsley, *Ergodic Theory and Information*, Wiley, New York, 1965.

In an important series of papers, D. Ornstein has clarified the extent to which entropy is a distinguishing invariant. The basic paper in the series is "Bernoulli Shifts with the Same Entropy are Isomorphic," *Advan. Math.* **4** (1970), 337–352.

PROBLEMS

*1. Let f be analytic in a neighborhood of $\sigma(A)$ where A is a bounded operator and let C be a contour as shown in Figure VII.3. Let $f(A)$ be defined by

$$f(A) = \frac{1}{2\pi i} \oint_C f(z)(z - A)^{-1}\, dz$$

Prove that $fg(A) = f(A)g(A)$.

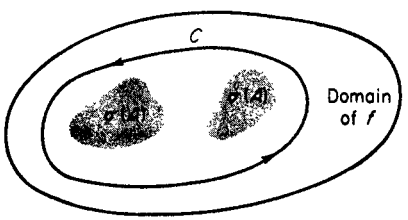

FIGURE VII.3 The contour C.

2. Suppose $\sigma(A)$ is not connected, say $\sigma(A) = \sigma_1 \cup \sigma_2$ where σ_1 and σ_2 are disjoint and closed. Consider the function f which is 1 in a neighborhood of σ_1 and 0 in a neighborhood of σ_2. Prove that $P = f(A)$ defined as in Problem 1 is a projection and that $PA = AP$. Prove that $\mathscr{H}_1 = \text{Ran } P$ is an invariant subspace for A and that $\sigma(A \restriction \mathscr{H}_1) = \sigma_1$.

3. (a) Prove that if A is **normal**, that is, $AA^* = A^*A$, then

$$\|A\| = \sup_{\lambda \in \sigma(A)} |\lambda| \equiv r(A)$$

Hint: Use $\|A\|^2 = \|A^*A\|$ and the formula $r(A) = \lim \|A^n\|^{1/n}$.

(b) Prove that for any polynomial P and any normal operator A, $\|P(A)\| = \sup_{\lambda \in \sigma(A)} |P(\lambda)|$.

*4. Let $A_1, \ldots, A_n$ be *commuting* bounded self-adjoint operators on $\mathscr{H}$, a separable Hilbert space.

(a) Let $\Omega_1, \ldots, \Omega_n$ be Borel sets on $\mathbb{R}$. Prove that $P_{\Omega_1}(A_1), P_{\Omega_2}(A_2), \ldots, P_{\Omega_n}(A_n)$ all commute.

(b) Let f be a function on $\mathbb{R}^n$ which is a linear combination of characteristic functions of rectangles (that is, sets of the form $\Omega = \Omega_1 \times \cdots \times \Omega_n$). Show that f can be written

$$f = \sum_{i=1}^{n} c_i \chi_{\Omega^{(i)}} \qquad \text{with} \quad \Omega^{(i)} \cap \Omega^{(j)} = \varnothing \quad \text{if} \quad i \neq j$$

(c) For f of the above form, define

$$f(A_1, \ldots, A_n) = \sum_{i=1}^{n} c_i P_{\Omega_1^{(i)}}(A_1) \cdots P_{\Omega_n^{(i)}}(A_n)$$

where $\Omega^{(i)} = \Omega_1^{(i)} \times \cdots \times \Omega_n^{(i)}$.

(d) By using the B.L.T. theorem, construct a continuous functional calculus, $f(A_1, \ldots, A_n)$ for continuous functions on $[-\|A_1\|, \|A_1\|] \times \cdots \times [-\|A_n\|, \|A_n\|]$.

(e) Construct a Borel functional calculus.

(f) Show there is a U: $\mathscr{H} \to L^2(M, d\mu)$ for some finite measure space $\langle M, \mu \rangle$ and bounded real-valued Borel functions $F_1(m), \ldots, F_n(m)$ on M with

$$[(UA_iU)^{-1}f](m) = F_i(m)f(m)$$

5. Let A be a normal operator. Prove:

(a) $A = B + iC$ where B and C are commuting self-adjoint operators.

(b) There is a U: $\mathscr{H} \to L^2(M, d\mu)$ for some finite measure μ on some space M and a bounded Borel function, $F(m)$ (in general, complex valued) so that

$$(UAU^{-1}f)(m) = F(m)f(m)$$

Reference for Problems 4, 5: Nelson (see the Notes to Section VII.1).

*6. Extend Problem 4 to the case of countably many A_n. *Hint*: Use the product topology on $X[-\|A_n\|, \|A_n\|]$.

†7. Find a self-adjoint operator A for which $[0, 1] \subset \sigma_{\text{sing}}(A)$ (*Hint*: Take A multiplicity free with a spectral measure which is an infinite weighted sum of translates of Cantor measures.)

†8. Let A be a bounded self-adjoint operator and let f be a continuous function on $\sigma(A)$.

(a) If $\lambda \notin \operatorname{Ran} f$, let $g = (f - \lambda)^{-1}$. Prove that $\phi(g) = (\phi(f) - \lambda)^{-1}$.

(b) Let $\lambda \in \operatorname{Ran} f(A)$. Prove that there are $\psi \in \mathscr{H}$, with $\|\psi\| = 1$ and $\|(\phi(f) - \lambda)\psi\|$ arbitrarily small so that $\lambda \in \sigma(\phi(f))$.

(c) Conclude (e) of Theorem VII.1.

†9. Suppose that f is continuous and f is not nonnegative on $\sigma(A)$ where A is a bounded self-adjoint operator. Show that there is a $\psi \in \mathscr{H}$ with $(\psi, \phi(f)\psi) < 0$.

†10. Prove that the range of the continuous functional calculus is the C^* algebra generated by A if A is self-adjoint (Theorem VII.1) or normal (Problem 5).

11. Suppose that $\phi: C(X) \to \mathscr{L}(\mathscr{H})$ is an algebraic $*$-homomorphism, X a compact Hausdorff space:
(a) Prove that $\phi(f) \geq 0$ if $f \geq 0$.
(b) Prove $\|\phi(f)\| \leq \|f\|_\infty$.

†12. Let $A \geq 0$. Prove that $(A - \lambda)^{-1}$ exists if $\lambda < 0$.

†13. Fill in the details of the proof of Theorem VII.2.

14. Prove that a self-adjoint operator on a finite-dimensional space has a cyclic vector if and only if it has no repeated eigenvalue.

†15. Prove Lemma 2 needed for Theorem VII.3.

16. Complete the reduction of Example 3 of Section VII.2 to a multiplication operator. Does this operator have uniform multiplicity? What is it?

†17. (a) Prove that $\sigma(A) = \text{supp } \{\mu_n\}_{n=1}^N$ if $\{\mu_n\}_{n=1}^N$ are the spectral measures. (The first proposition after Theorem VII.3.)
(b) Let T_F be the operator of multiplications by F, a real-valued bounded measurable function. Prove that $\sigma(T_F)$ is the essential range of F.

†18. Let A be multiplication by x on $L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{ac}) \oplus L^2(\mathbb{R}, d\mu_{pp}) \oplus L^2(\mathbb{R}, d\mu_{sing})$. Let $\psi \in L^2(\mathbb{R}, d\mu)$. Prove that $d\mu_\psi$ is absolutely continuous if and only if $\psi \in L^2(\mathbb{R}, d\mu_{ac})$.

*19. Is it possible to have a measure on [0, 1] absolutely continuous w.r.t. dx with support [0, 1] but which is not equivalent to dx, that is, is supp $\langle\mu\rangle$ a distinguishing invariant for measure classes absolutely continuous w.r.t. dx?

20. Let $A = U|A|$ be the polar decomposition of A. Let f_n be defined by $f_n(x) = 1/x$ if $x \geq 1/n$ and $f_n(x) = 1/n$ if $x \leq 1/n$. Prove that $U = \text{s-lim } Af_n(|A|)$. Conclude that U is in the von Neumann algebra generated by A, that is, the smallest strongly closed $*$-algebra containing A.

†21. (a) Prove that conditions (a) and (b) of Theorem VII.5 are equivalent.
*(b) Prove condition (a) of Theorem VII.5 implies condition (c) in general. (*Hint*: Prove that $\{B \mid AB = BA\} = L^\infty(M, d\mu)$.)
(c) Prove (c) implies (a) in the finite-dimensional case.

†22. (a) Prove that the properties (a)–(d) of a p.v.m. hold for the spectral projections of an operator A.
(b) Prove that condition (d) for a p.v.m. follows from (a) and (c).

†23. (a) Supply the details of the proof of Theorem VII.7.
(b) Prove that $f(A) = \int f(\lambda)\, dP_\lambda$ if $P_\Omega = \chi_\Omega(A)$.
(c) If $A = \int \lambda\, dP_\lambda$, prove that $P_\Omega = \chi_\Omega(A)$.

†24. Prove $\lambda \in \sigma(A)$ if and only if $P_{(\lambda-\varepsilon, \lambda+\varepsilon)}(A) \neq 0$ for all ε.

25. By considering compact operators, prove that σ_{disc} is not always closed.

†26. (a) Prove Theorem VII.10.
(b) Prove Theorem VII.11.

27. Let C be self-adjoint and compact. What is $\sigma_{\text{ess}}(C)$? How is this related to the invariance property of σ_{ess} described at the end of Section VIII.3?

28. (a) Suppose that μ is a measure of unit mass with the property: Given $0 < x < 1$, there is a set $N \subset M$ with $\mu(N) = x$. Let $T: M \to M$ be measure preserving with $T^k = I$ for some k. Prove that T is not ergodic.
(b) Prove directly that $T_{a,b}$ of Example 1 of Section VII.4 is not ergodic if $na + mb = r$ has a solution with r integral and $\langle n, m\rangle \neq \langle 0, 0\rangle$ (that is, without recourse to the unitary U).

29. Show that the following measurable transformations are all equivalent to the Baker's transformation:
(a) $M = \times_{n=-\infty}^{\infty} A_n$ where each A_n is the two-point set $\{H_n, T_n\} = A_n$[Heads, Tails]. μ is the product measure $\mu = \otimes_{n=-\infty}^{\infty} \mu_n$ where $\mu_n(\{H_n\}) = \frac{1}{2} = \mu_n(\{T_n\})$. Let $T: M \to M$ by shifting to the right. (This is called the honest coin toss space.)
(b) $M = \times_{n=-\infty}^{\infty} B_n$ where each B_n is the three-point space, $B = \{0, 1, 2\}$. μ is the product measure $\mu = \otimes_{n=-\infty}^{\infty} \nu_n$ where $\nu_0(\{0\}) = \frac{1}{2} = \nu_n(\{2\})$; $\nu_n(\{1\}) = 0$. T is a right shift.
(c) M is the square with the product of the Cantor measure with itself. T is given by

$$T\langle x, y\rangle = \begin{cases} \langle 3x, \frac{1}{3}y\rangle & \text{if } 0 \leq x < \frac{1}{3} \\ \langle 3x - 1, \frac{1}{3}y + \frac{1}{3}\rangle & \text{if } \frac{1}{3} \leq x < \frac{2}{3} \\ \langle 3x - 2, \frac{1}{3}y + \frac{2}{3}\rangle & \text{if } \frac{2}{3} \leq x < 1 \end{cases}$$

30. Let $\langle M, \mu\rangle$ be a measure space with $T: M \to M$. Define $T \otimes T: M \times M \to M \times M$ by $(T \otimes T)\langle x, y\rangle = \langle Tx, Ty\rangle$.
(a) Show that $\mu \otimes \mu$ is an invariant measure for $T \otimes T$ if μ is an invariant measure for T.
(b) Find an example which shows that $T \otimes T$ may be not ergodic for $\langle M \times M, \mu \otimes \mu\rangle$ even if T is ergodic for $\langle M, \mu\rangle$. [*Hint*: Look at Example 1 of Section VII.4.]
(c) Show that $T \otimes T$ is mixing for $\langle M \times M, \mu \otimes \mu\rangle$ if T is mixing for $\langle M, \mu\rangle$.
(d) Show, once more, that Example 1 is not mixing by using (c).
Remark: It is known that $T \otimes T$ is ergodic if and only if T is weakly mixing.

31. Prove that the only closed $*$-ideals in $\mathscr{L}(\mathscr{H})$, where $\mathscr{H}$ is separable, are $\{0\}$, $\text{Com}(\mathscr{H})$, and $\mathscr{L}(\mathscr{H})$. *Hint*: If the ideal $\mathscr{I}$ strictly contains $\text{Com}(\mathscr{H})$, find a self-adjoint, noncompact, operator $A \in \mathscr{I}$. Show that for any interval (a, b), with $0 \notin (a, b)$, $P_{(a,b)}(A) \in \mathscr{I}$. Conclude that $\mathscr{I}$ contains an infinite-dimensional projection and thus that $I \in \mathscr{I}$.

32. (a) Let A be self-adjoint and let U_λ be the partial isometry in $U_\lambda |A - \lambda| = A - \lambda$. Prove that $U_\lambda = P_{(\lambda, \infty)} - P_{(-\infty, \lambda)}$ and that $P_{(-\infty, \lambda)} = \lim_{\mu \uparrow \lambda} \frac{1}{2}(1 - U_\mu)$ and $P_{(-\infty, \lambda]} = \lim_{\mu \downarrow \lambda} \frac{1}{2}(1 - U_\mu)$.
(b) Given a self-adjoint operator, use the polar decomposition and the formula of (a) to prove the spectral theorem without recourse to the functional calculus.

VIII: Unbounded Operators

I tell them that if they will occupy themselves with the study of mathematics they will find in it the best remedy against the lusts of the flesh. *Thomas Mann in* ***The Magic Mountain***

VIII.1 Domains, graphs, adjoints, and spectrum

It is a fact of life that many of the most important operators which occur in mathematical physics are not bounded. In this chapter we will introduce some of the basic definitions and theorems necessary for dealing with unbounded operators on Hilbert spaces. The Hellinger–Toeplitz theorem (see Section III.5) says that an everywhere-defined operator A which satisfies $(A\varphi, \psi) = (\varphi, A\psi)$ is necessarily a bounded operator suggesting that a general unbounded operator T will only be defined on a dense linear subset of the Hilbert space $\mathscr{H}$. Thus an **operator** on a Hilbert space $\mathscr{H}$ is a linear map from its domain, a linear subspace of $\mathscr{H}$, into $\mathscr{H}$. Unless we specify otherwise, we will always suppose that the domain is dense. This subspace, which we denote by $D(T)$, is called the **domain** of the operator T. So, to identify an unbounded operator on a Hilbert space one must first give the domain on which it acts and then specify how it acts on that subspace.

Example 1 (the position operator) Let $\mathscr{H} = L^2(\mathbb{R})$ and let $D(T)$ be the set of functions φ in $L^2(\mathbb{R})$ which satisfy $\int_{\mathbb{R}} x^2 |\varphi(x)|^2 \, dx < \infty$. For $\varphi \in D(T)$ define $(T\varphi)(x) = x\varphi(x)$. It is clear that T is unbounded since if we choose φ to

have support near plus or minus infinity, we can make $\|T\varphi\|$ as large as we like while keeping $\|\varphi\| = 1$. Of course, even if $\varphi \notin D(T)$, $x\varphi(x)$ has a well-defined meaning as a function, but it is not in $L^2(\mathbb{R})$. Thus, if we want to deal only with the Hilbert space $L^2(\mathbb{R})$ we must restrict the domain of T. The domain we have chosen is the largest one for which the range is in $L^2(\mathbb{R})$.

Example 2 Let $\mathscr{H} = L^2(\mathbb{R})$ and $D(T) = \mathscr{S}(\mathbb{R})$. On $D(T)$ define $T\psi = -\psi''(x) + x^2\psi(x)$. If $\varphi_n(x)$ is the nth Hermite function (see the appendix to Section V.3), then $\varphi_n(x) \in D(T)$ and $T\varphi_n(x) = (2n + 1)\varphi_n(x)$. Thus T must be unbounded since it has arbitrarily large eigenvalues.

The notion of the graph of a linear transformation, introduced by von Neumann, is very useful for studying unbounded operators.

Definition The **graph** of the linear transformation T is the set of pairs

$$\{\langle \varphi, T\varphi\rangle \mid \varphi \in D(T)\}$$

The graph of T, denoted by $\Gamma(T)$, is thus a subset of $\mathscr{H} \times \mathscr{H}$ which is a Hilbert space with inner product

$$(\langle \varphi_1, \psi_1\rangle, \langle \varphi_2, \psi_2\rangle) = (\varphi_1, \varphi_2) + (\psi_1, \psi_2)$$

T is called a **closed** operator if $\Gamma(T)$ is a closed subset of $\mathscr{H} \times \mathscr{H}$.

Definition Let T_1 and T be operators on $\mathscr{H}$. If $\Gamma(T_1) \supset \Gamma(T)$, then T_1 is said to be an **extension** of T and we write $T_1 \supset T$. Equivalently, $T_1 \supset T$ if and only if $D(T_1) \supset D(T)$ and $T_1\varphi = T\varphi$ for all $\varphi \in D(T)$.

Definition An operator T is **closable** if it has a closed extension. Every closable operator has a smallest closed extension, called its **closure**, which we denote by $\overline{T}$.

A natural way to try to obtain a closed extension of an operator, T, is to take the closure of its graph in $\mathscr{H} \times \mathscr{H}$. The trouble with this is that $\overline{\Gamma(T)}$ may not be the graph of an operator (for example, see Problem 1). However, most operators which we deal with will be symmetric operators (introduced in Section VIII.2) and we will see that they always have closed extensions.

Proposition If T is closable, then $\Gamma(\overline{T}) = \overline{\Gamma(T)}$.

Proof Suppose that S is a closed extension of T. Then $\overline{\Gamma(T)} \subset \Gamma(S)$ so if $\langle 0, \psi\rangle \in \overline{\Gamma(T)}$ then $\psi = 0$. Define R with $D(R) = \{\psi \mid \langle \psi, \phi\rangle \in \overline{\Gamma(T)}$ for some

$\phi\}$ by $R\psi = \phi$ where $\phi \in \mathscr{H}$ is the unique vector so that $\langle \psi, \phi \rangle \in \overline{\Gamma(T)}$. Then $\Gamma(R) = \overline{\Gamma(T)}$ so R is a closed extension of T. But $R \subset S$ which is an arbitrary closed extension, so $R = \bar{T}$. ∎

The following example illustrates the concepts we have just introduced.

Example 3 Let $\mathscr{H} = L^2(\mathbb{R})$, $D(T) = C_0^\infty(\mathbb{R})$, and $D(T_1) = C_0^1(\mathbb{R})$, the once continuously differentiable functions with compact support. Let $Tf = if'(x)$ if $f \in D(T)$ and $T_1 f = if'(x)$ if $f \in D(T_1)$. T_1 is an extension of T. We will show that $\overline{\Gamma(T)} \supset \Gamma(T_1)$. When we prove that T is symmetric and therefore closable, it will follow that $\bar{T}$ extends T_1. First we introduce the approximate identity, $\{j_\varepsilon(x)\}$. Let $j(x)$ be any positive, infinitely differentiable function with support in $(-1, 1)$ so that $\int_{-\infty}^{\infty} j(x)\,dx = 1$. Define $j_\varepsilon(x) = \varepsilon^{-1} j(x/\varepsilon)$. If $\varphi \in D(T_1)$, set

$$\varphi_\varepsilon(x) = \int_{-\infty}^{\infty} j_\varepsilon(x - t)\varphi(t)\,dt$$

Then

$$\begin{aligned} |\varphi_\varepsilon(x) - \varphi(x)| &\leq \int j_\varepsilon(x - t)|\varphi(t) - \varphi(x)|\,dt \\ &\leq \left(\sup_{\{t \mid |x-t| \leq \varepsilon\}} |\varphi(t) - \varphi(x)| \right) \int_{\mathbb{R}} j_\varepsilon(x - t)\,dt \\ &= \sup_{\{t \mid |x-t| \leq \varepsilon\}} |\varphi(t) - \varphi(x)| \end{aligned}$$

Since φ has compact support, it is uniformly continuous which implies that $\varphi_\varepsilon \to \varphi$ uniformly. Since the φ_ε have support in a fixed compact set, $\varphi_\varepsilon \to \varphi$ in $L^2(\mathbb{R})$. Similarly,

$$\begin{aligned} i\frac{d}{dx}\varphi_\varepsilon(x) &= \int_{-\infty}^{\infty} i\frac{d}{dx} j_\varepsilon(x - t)\varphi(t)\,dt \\ &= \int_{-\infty}^{\infty} -i\left(\frac{d}{dt} j_\varepsilon(x - t)\right)\varphi(t)\,dt \\ &= \int_{-\infty}^{\infty} j_\varepsilon(x - t) i\frac{d}{dt}\varphi(t)\,dt \\ &\xrightarrow{L^2(\mathbb{R})} i\frac{d}{dx}\varphi(x) \end{aligned}$$

Since $j_\varepsilon(x)$ has compact support and is infinitely differentiable, $\varphi_\varepsilon \in C_0^\infty(\mathbb{R})$. Thus, $\varphi_\varepsilon \in D(T)$ for each $\varepsilon > 0$. What we have shown above is that $\varphi_\varepsilon \xrightarrow{L^2(\mathbb{R})} \varphi$ and $T\varphi_\varepsilon \xrightarrow{L^2(\mathbb{R})} T_1\varphi$ for any $\varphi \in D(T_1)$. Thus, the closure of the graph of T contains the graph of T_1.

The notion of adjoint operator can be extended to the unbounded case.

Definition Let T be a densely defined linear operator on a Hilbert space $\mathscr{H}$. Let $D(T^*)$ be the set of $\varphi \in \mathscr{H}$ for which there is an $\eta \in \mathscr{H}$ with

$$(T\psi, \varphi) = (\psi, \eta) \qquad \text{for all} \quad \psi \in D(T) \tag{VIII.1}$$

For each such $\varphi \in D(T^*)$, we define $T^*\varphi = \eta$. T^* is called the **adjoint** of T. By the Riesz lemma, $\varphi \in D(T^*)$ if and only if $|(T\psi, \varphi)| \leq C\|\psi\|$ for all $\psi \in D(T)$.

We note that $S \subset T$ implies $T^* \subset S^*$.

Notice that for η to be uniquely determined by (VIII.1) we need the fact that $D(T)$ is dense. Unlike the case of bounded operators, the domain of T^* may not be dense as the following example shows. As a matter of fact it is possible to have $D(T^*) = \{0\}$.

Example 4 Suppose that f is a bounded measurable function, but that $f \notin L^2(\mathbb{R})$. Let $D(T) = \{\psi \in L^2(\mathbb{R}) \mid \int |f(x)\psi(x)|\, dx < \infty\}$. $D(T)$ certainly contains all the L^2 functions with compact support so $D(T)$ is dense in $L^2(\mathbb{R})$. Let ψ_0 be some fixed vector in $L^2(\mathbb{R})$ and define $T\psi = (f, \psi)\psi_0$ for $\psi \in D(T)$. Suppose that $\varphi \in D(T^*)$, then

$$\begin{aligned}(\psi, T^*\varphi) = (T\psi, \varphi) &= ((f, \psi)\psi_0, \varphi) \\ &= \overline{(f, \psi)}(\psi_0, \varphi) \\ &= (\psi, (\psi_0, \varphi)f)\end{aligned}$$

for all $\psi \in D(T)$. Thus $T^*\varphi = (\psi_0, \varphi)f$. Since $f \notin L^2(\mathbb{R})$, $(\psi_0, \varphi) = 0$. Thus any $\varphi \in D(T^*)$, is orthogonal to ψ_0, so $D(T^*)$ is not dense. In fact, $D(T^*)$ is just the vectors perpendicular to ψ_0, and on that domain T^* is the zero operator.

If the domain of T^* is dense, then we can define $T^{**} = (T^*)^*$. There is a simple relationship between the notions of adjoint and closure.

Theorem VIII.1 Let T be a densely defined operator on a Hilbert space $\mathscr{H}$. Then:

(a) T^* is closed.
(b) T is closable if and only if $D(T^*)$ is dense in which case $\overline{T} = T^{**}$.
(c) If T is closable, then $(\overline{T})^* = T^*$.

Proof We define a unitary operator V on $\mathscr{H} \times \mathscr{H}$ by

$$V\langle \phi, \psi \rangle = \langle -\psi, \phi \rangle$$

Since V is unitary, $V[E^\perp] = (V[E])^\perp$ for any subspace E. Let T be a linear operator on $\mathscr{H}$ and suppose $\langle \phi, \eta \rangle \in \mathscr{H} \times \mathscr{H}$. Then $\langle \phi, \eta \rangle \in V[\Gamma(T)]^\perp$ if and only if $(\langle \phi, \eta \rangle, \langle -T\psi, \psi \rangle) = 0$ for all $\psi \in D(T)$ which holds if and only if $(\phi, T\psi) = (\eta, \psi)$ for all $\psi \in D(T)$, that is, if and only if $\langle \phi, \eta \rangle \in \Gamma(T^*)$. Thus $\Gamma(T^*) = V[\Gamma(T)]^\perp$. Since $V[\Gamma(T)]^\perp$ is always a closed subspace of $\mathscr{H} \times \mathscr{H}$, this proves (a).

To prove (b), observe that $\Gamma(T)$ is a linear subset of $\mathscr{H} \times \mathscr{H}$ so

$$\begin{aligned} \overline{\Gamma(T)} &= (\Gamma(T)^\perp)^\perp \\ &= (V^2\Gamma(T)^\perp)^\perp \\ &= (V(V\Gamma(T))^\perp)^\perp \\ &= (V\Gamma(T^*))^\perp \end{aligned}$$

Thus, by the proof of (a), if T^* is densely defined, $\overline{\Gamma(T)}$ is the graph of T^{**}.

Conversely, suppose that $D(T^*)$ is not dense and that $\psi \in D(T^*)^\perp$. A simple computation shows that $\langle \psi, 0 \rangle \in [\Gamma(T^*)]^\perp$ so $V[\Gamma(T^*)]^\perp$ is not the graph of a (single-valued) operator. Since $\overline{\Gamma(T)} = (V\Gamma(T^*))^\perp$, we see that T is not closable.

To prove (c), notice that if T is closable,

$$T^* = \overline{(T^*)} = T^{***} = (\overline{T})^* \quad \blacksquare$$

Definition Let T be a closed operator on a Hilbert space $\mathscr{H}$. A complex number λ is in the **resolvent set**, $\rho(T)$, if $\lambda I - T$ is a bijection of $D(T)$ onto $\mathscr{H}$ with a bounded inverse. If $\lambda \in \rho(T)$, $R_\lambda(T) = (\lambda I - T)^{-1}$ is called the **resolvent** of T at λ.

For a point to be in the resolvent set of T, several conditions must be satisfied. These conditions are not all independent. For example, if $\lambda I - T$ is a bijection of $D(T)$ onto $\mathscr{H}$, by the closed-graph theorem, its inverse is automatically bounded. For other relationships, see Problem 2.

The definitions of **spectrum**, **point spectrum**, and **residual spectrum** are the same for unbounded operators as they are for bounded operators. We will sometimes refer to the spectrum of nonclosed, but closable operators. In this case we always mean the spectrum of the closure.

Theorem VIII.2 Let T be a closed densely defined linear operator. Then the resolvent set of T is an open subset of the complex plane on which the resolvent is an analytic operator-valued function. Furthermore,

$$\{R_\lambda(T) \mid \lambda \in \rho(T)\}$$

is a commuting family of bounded operators satisfying

$$R_\lambda(T) - R_\mu(T) = (\mu - \lambda)R_\mu(T)R_\lambda(T) \tag{VIII.2}$$

The proof of this theorem is exactly the same as the proof of the bounded case (Theorem VI.5).

It may seem to the reader that many of the questions about domains and closures of unbounded operators are just a technical inconvenience; that one need only choose any dense domain which is small enough so that the unbounded operator makes sense and that is good enough. However, the choice of an appropriate domain is often intimately connected with the physics of the situation being described; see, for example, the discussion in Section X.1. Further, many of the properties of operators which are important are very sensitive to the choice of domain. The following example shows that the spectrum is such a property. In the example we use the notion of "absolutely continuous function" and the corresponding fundamental theorem of calculus. The reader who is unfamiliar with the definition and theorem can find them in the notes.

Example 5 We denote by $AC[0, 1]$ the set of absolutely continuous functions on $[0, 1]$ whose derivatives are in $L^2[0, 1]$. Let T_1 and T_2 be the operation $i\,d/dx$ with domains

$$D(T_1) = \{\varphi \mid \varphi \in AC[0, 1]\}$$
$$D(T_2) = \{\varphi \mid \varphi \in AC[0, 1] \quad \text{and} \quad \varphi(0) = 0\}$$

Both $D(T_1)$ and $D(T_2)$ are dense in $L^2[0, 1]$ and both of the operators are closed. But:

(a) The spectrum of T_1 is $\mathbb{C}$.
(b) The spectrum of T_2 is empty.

The proof that T_1 and T_2 are closed is left as an exercise (Problem 3). To see that the spectrum of T_1 is the whole plane we observe that

$$(\lambda I - T_1)e^{-i\lambda x} = 0 \qquad \text{and} \qquad e^{-i\lambda x} \in D(T_1)$$

for all $\lambda \in \mathbb{C}$. As for T_2, the operator

$$(S_\lambda g)(x) = i \int_0^x e^{-i\lambda(x-s)} g(s)\, ds$$

satisfies $(\lambda I - T_2)S_\lambda = I$ and $S_\lambda(\lambda I - T_2)$ is the identity on $D(T_2)$. Moreover,

$$\begin{aligned}\|S_\lambda g\|_2^2 &= \int_0^1 |(S_\lambda g)(x)|^2\, dx \\ &\leq \left(\sup_{x\in[0,1]} |(S_\lambda g)(x)|\right)^2 \\ &\leq \left(\sup_{x\in[0,1]} \int_0^x |e^{-i\lambda(x-s)}g(s)|\, ds\right)^2 \\ &\leq \left(\sup_{x\in[0,1]} \left(\int_0^x |e^{-i\lambda(x-s)}|^2\, ds\right)\right)\left(\sup_{x\in[0,1]} \int_0^x |g(s)|^2\, ds\right) \\ &\leq C(\lambda)\, \|g\|_2^2\end{aligned}$$

so S_λ is bounded. By the remark immediately after the definition of resolvent set, we need only have shown that $\lambda I - T_2$ is a bijection to conclude that S_λ is bounded. So, we could have avoided the above computation.

VIII.2 Symmetric and self-adjoint operators: the basic criterion for self-adjointness

Definition A densely defined operator T on a Hilbert space is called **symmetric** (or **Hermitian**) if $T \subset T^*$, that is, if $D(T) \subset D(T^*)$ and $T\varphi = T^*\varphi$ for all $\varphi \in D(T)$. Equivalently, T is symmetric if and only if

$$(T\varphi, \psi) = (\varphi, T\psi) \qquad \text{for all} \quad \varphi, \psi \in D(T)$$

Definition T is called **self-adjoint** if $T = T^*$, that is, if and only if T is symmetric and $D(T) = D(T^*)$.

A symmetric operator is always closable, since $D(T^*) \supset D(T)$ is dense in $\mathscr{H}$. If T is symmetric, T^* is a closed extension of T, so the smallest closed extension T^{**} of T must be contained in T^*. Thus for symmetric operators, we have

$$T \subset T^{**} \subset T^*$$

For closed symmetric operators,

$$T = T^{**} \subset T^*$$

And, for self-adjoint operators,

$$T = T^{**} = T^*$$

From this one can easily see that a closed symmetric operator T is self-adjoint if and only if T^* is symmetric.

The distinction between closed symmetric operators and self-adjoint operators is very important. It is only for *self-adjoint* operators that the spectral theorem holds (see Section VIII.3) and it is only *self-adjoint* operators that may be exponentiated to give the one-parameter unitary groups (see Section VIII.4) which give the dynamics in quantum mechanics. Chapter X is mainly devoted to studying methods for proving that operators are self-adjoint. We content ourselves here with proving the basic criterion for self-adjointness. First, we introduce the useful notion of essential self-adjointness.

Definition A symmetric operator T is called **essentially self-adjoint** if its closure $\overline{T}$ is self-adjoint. If T is closed, a subset $D \subset D(T)$ is called a **core** for T if $\overline{T \restriction D} = T$.

If T is essentially self-adjoint, then it has one and only one self-adjoint extension, for suppose that S is a self-adjoint extension of T. Then, S is closed and thereby, since $S \supset T$, $S \supset T^{**}$. Thus, $S = S^* \subset (T^{**})^* = T^{**}$, and so $S = T^{**}$. The converse is also true; namely, if T has one and only one self-adjoint extension, then T is essentially self-adjoint (see Section X.1). Since $T^* = \overline{T}^* = T^{***}$, T is essentially self-adjoint if and only if

$$T \subset T^{**} = T^*$$

The importance of essential self-adjointness is that one is often given a nonclosed symmetric operator T. If T can be shown to be essentially self-adjoint, then there is uniquely associated to T a self-adjoint operator $\overline{T} = T^{**}$. Another way of saying this is that if A is a self-adjoint operator, then to specify A uniquely one need not give the exact domain of A (which is often difficult), but just some core for A.

Now, suppose that T is a self-adjoint operator and that there is a $\varphi \in D(T^*) = D(T)$ so that $T^* \varphi = i\varphi$. Then $T\varphi = i\varphi$ and

$$-i(\varphi, \varphi) = (i\varphi, \varphi) = (T\varphi, \varphi) = (\varphi, T^*\varphi) = (\varphi, T\varphi) = i(\varphi, \varphi)$$

so $\varphi = 0$. A similar proof shows that $T^*\varphi = -i\varphi$ can have no solutions. The converse statement, that if T is a closed symmetric operator and $T^*\varphi = \pm i\varphi$ has no solutions, then T is self-adjoint, is the basic criterion of self-adjointness.

Theorem VIII.3 (the basic criterion for self-adjointness) Let T be a symmetric operator on a Hilbert space $\mathscr{H}$. Then the following three statements are equivalent:

(a) T is self-adjoint.
(b) T is closed and $\mathrm{Ker}(T^* \pm i) = \{0\}$.
(c) $\mathrm{Ran}(T \pm i) = \mathscr{H}$.

Proof We have just seen that (a) implies (b). Suppose that (b) holds; we will prove (c). Since $T^*\varphi = -i\varphi$ has no solutions, $\mathrm{Ran}(T - i)$ must be dense. Otherwise, if $\psi \in \mathrm{Ran}(T - i)^{\perp}$, we would have $((T - i)\varphi, \psi) = 0$ for all $\varphi \in D(T)$, so $\psi \in D(T^*)$ and $(T - i)^*\psi = (T^* + i)\psi = 0$ which is impossible since $T^*\psi = -i\psi$ has no solutions. (Reversing this last argument we can show that if $\mathrm{Ran}(T - i)$ is dense, the kernel of $T^* + i$ is $\{0\}$.) Since $\mathrm{Ran}(T - i)$ is dense, we need only prove it is closed to conclude that $\mathrm{Ran}(T - i) = \mathscr{H}$. But for all $\varphi \in D(T)$

$$\|(T - i)\varphi\|^2 = \|T\varphi\|^2 + \|\varphi\|^2$$

Thus if $\varphi_n \in D(T)$ and $(T - i)\varphi_n \to \psi_0$, we conclude that φ_n converges to some vector φ_0, and $T\varphi_n$ converges too. Since T is closed, $\varphi_0 \in D(T)$ and $(T - i)\varphi_0 = \psi_0$. Thus, $\mathrm{Ran}(T - i)$ is closed, so $\mathrm{Ran}(T - i) = \mathscr{H}$. Similarly, $\mathrm{Ran}(T + i) = \mathscr{H}$.

Finally, we will show that (c) implies (a). Let $\varphi \in D(T^*)$. Since $\mathrm{Ran}(T - i) = \mathscr{H}$, there is an $\eta \in D(T)$ so that $(T - i)\eta = (T^* - i)\varphi$. $D(T) \subset D(T^*)$, so $\varphi - \eta \in D(T^*)$ and

$$(T^* - i)(\varphi - \eta) = 0$$

Since $\mathrm{Ran}(T + i) = \mathscr{H}$, $\mathrm{Ker}(T^* - i) = \{0\}$, so $\varphi = \eta \in D(T)$. This proves that $D(T^*) = D(T)$, so T is self-adjoint. ∎

Corollary Let T be a symmetric operator on a Hilbert space. Then the following are equivalent:

(a) T is essentially self-adjoint.
(b) $\mathrm{Ker}(T^* \pm i) = \{0\}$.
(c) $\mathrm{Ran}(T \pm i)$ are dense.

We conclude with an example which shows that a symmetric operator may have many self-adjoint extensions. Lest the reader be misled we remark that a symmetric operator may have *no* self-adjoint extensions (see Problem 4 and Section X.1).

Example Let $T = i\,d/dx$ with

$$D(T) = \{\varphi \mid \varphi \in AC[0, 1], \quad \varphi(0) = 0 = \varphi(1)\}$$

A simple integration by parts shows that as an operator on $L^2[0, 1]$, T is symmetric. We begin by determining T^*. Let j_ε be the function defined in

Example 3 of Section VIII.1. Fix $0 < \alpha < \beta < 1$ and define

$$f_\varepsilon^{\alpha,\beta}(x) = j_\varepsilon(x - \beta) - j_\varepsilon(x - \alpha)$$

$$g_\varepsilon^{\alpha,\beta}(x) = \int_0^x f_\varepsilon^{\alpha,\beta}(t)\, dt$$

Let $\psi \in D(T^*)$. For ε small enough, $g_\varepsilon^{\alpha,\beta} \in D(T)$ so

$$(Tg_\varepsilon^{\alpha,\beta}, \psi) = (g_\varepsilon^{\alpha,\beta}, T^*\psi) \qquad \text{(VIII.3)}$$

As $\varepsilon \to 0$, $-g_\varepsilon^{\alpha,\beta}$ converges to the characteristic function of (α, β) in $L^2(0, 1)$ so

$$(g_\varepsilon^{\alpha,\beta}, T^*\psi) \to -\int_\alpha^\beta (T^*\psi)(x)\, dx$$

The basic estimate of Example 3 shows that

$$J_\varepsilon \varphi = \int_0^1 j_\varepsilon(x - t)\varphi(t)\, dt$$

converges in L^2 to φ if φ is continuous. Moreover, each J_ε is a bounded operator of norm not greater than one. For if $\psi \in L^2(0, 1)$, then

$$\begin{aligned} |(\psi, J_\varepsilon \varphi)| &\le \iint j_\varepsilon(x - t)|\varphi(t)|\ |\psi(x)|\ dx\, dt \\ &= \iint j_\varepsilon(y)|\varphi(t)|\ |\psi(y + t)|\ dy\, dt \\ &\le \|\varphi\|\, \|\psi\| \int j_\varepsilon(y)\, dy \\ &= \|\varphi\|\, \|\psi\| \end{aligned}$$

By an $\varepsilon/3$ argument, $J_\varepsilon \varphi \xrightarrow{L^2} \varphi$ for all $\varphi \in L^2[0, 1]$. Thus, the left side of (VIII.3) converges to $-i(\psi(\beta) - \psi(\alpha))$ in mean square as $\varepsilon \to 0$. So, for almost all α, β

$$i(\psi(\beta) - \psi(\alpha)) = \int_\alpha^\beta (T^*\psi)(x)\, dx$$

This means that ψ is absolutely continuous (see the Notes for Section VIII.1) and

$$i\frac{d}{dx}\psi(x) = (T^*\psi)(x)$$

Thus, $\psi \in AC[0, 1]$ and $T^*\psi = i\, d\psi(x)/dx$. Conversely, integration by parts shows that any $\psi \in AC[0, 1]$ is in the domain of T^* and $T^*\psi = i\, d\psi/dx$. Therefore $T^* = i\, d/dx$ on $D(T^*) = AC[0, 1]$.

It is easy to see that T is not essentially self-adjoint since

$$e^{\pm x} \in D(T^*) \qquad \text{and} \qquad i\frac{d}{dx}e^{\pm x} = \pm ie^{\pm x}$$

In fact, T is closed (Problem 6) so T is a closed, symmetric but not self-adjoint operator.

Does T have any self-adjoint extensions? Yes, uncountably many different ones! Let $\alpha \in \mathbb{C}$, $|\alpha| = 1$, and define $T_\alpha = i\,d/dx$ on

$$D(T_\alpha) = \{\varphi \mid \varphi \in AC[0, 1], \quad \varphi(0) = \alpha\varphi(1)\}$$

Each of these operators T_α is a different self-adjoint extension of T (Problem 7). Of course, each T_α is in turn extended by T^*. These extensions are depicted in Figure VIII.1. The reason why there is exactly a circle of different possible extensions will be made clear in Section X.1.

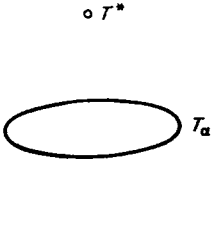

FIGURE VIII.1 The self-adjoint extensions of T.

VIII.3 The spectral theorem

A good definition should be the hypothesis of a theorem. *J. Glimm*

In this section we will show how the spectral theorem for bounded self-adjoint operators which we developed in Chapter VII can be extended to unbounded self-adjoint operators. To indicate what we are aiming for, we first prove the following:

Proposition 1 Let $\langle M, \mu\rangle$ be a measure space with μ a finite measure. Suppose that f is a measurable, real-valued function on M which is finite a.e.$[\mu]$. Then the operator $\varphi \xrightarrow{T_f} f\varphi$ on $L^2(M, d\mu)$ with domain

$$D(T_f) = \{\varphi \mid f\varphi \in L^2(M, \mu)\}$$

is self-adjoint and $\sigma(T_f)$ is the essential range of f.

Proof T_f is clearly symmetric. Suppose that $\psi \in D(T_f^*)$ and let

$$\chi_N(m) = \begin{cases} 1 & \text{if } |f(m)| \leq N \\ 0 & \text{otherwise} \end{cases}$$

Then, using the monotone convergence theorem,

$$\begin{aligned}\|T_f^*\psi\| &= \lim_{N\to\infty} \|\chi_N T_f^*\psi\| \\ &= \lim_{N\to\infty} \left(\sup_{\|\varphi\|=1} |(\varphi, \chi_N T_f^*\psi)| \right) \\ &= \lim_{N\to\infty} \left(\sup_{\|\varphi\|=1} |(T_f \chi_N \varphi, \psi)| \right) \\ &= \lim_{N\to\infty} \left(\sup_{\|\varphi\|=1} |(\varphi, \chi_N f\psi)| \right) \\ &= \lim_{N\to\infty} \|\chi_N f\psi\|\end{aligned}$$

Thus, $f\psi \in L^2(M, \mu)$, so $\psi \in D(T_f)$ and therefore T_f is self-adjoint. That $\sigma(T_f)$ is the essential range of f follows as in the bounded case (Problem 17 of Chapter VII). ∎

With more information about f, one can say something about the domains on which T_f is essentially self-adjoint:

Proposition 2 Let f and T_f obey the conditions in Proposition 1. Suppose in addition that $f \in L^p(M, d\mu)$ for $2 < p < \infty$. Let D be any dense set in $L^q(M, d\mu)$ where $q^{-1} + p^{-1} = 1/2$. Then D is a core for T_f.

Proof Let us first show that L^q is a core for T_f. By Holder's inequality $\|g\|_2 \leq \|1\|_p \|g\|_q$ and $\|fg\|_2 \leq \|f\|_p \|g\|_q$ so $L^q \subset D(T_f)$. Moreover, if $g \in D(T_f)$, let g_n be that function which is zero where $|g(m)| > n$ and equal to g otherwise. By the dominated convergence theorem, $g_n \to g$ and $fg_n \to fg$ in L^2. Since each g_n is in L^q, we conclude that L^q is a core for T_f.

Now let D be dense in L^q and let $g \in L^q$. Find $g_n \in D$ with $g_n \to g$ in L^q. Since $\|g_n - g\|_2 \leq \|1\|_p \|g_n - g\|_q$ and $\|T_f(g_n - g)\|_2 \leq \|f\|_p \|g_n - g\|_q$, $g \in D(\overline{T_f \restriction D})$. Thus $L^q \subset D(\overline{T_f \restriction D})$ so D is a core. ∎

Unless $f \in L^\infty(M, \mu)$ the operator T_f described in Propositions 1 and 2 will be unbounded. Thus, we have found a large class of unbounded self-adjoint operators. In fact, we have found them all.

Theorem VIII.4 (spectral theorem—multiplication operator form) Let A be a self-adjoint operator on a separable Hilbert space $\mathscr{H}$ with domain $D(A)$. Then there is a measure space $\langle M, \mu\rangle$ with μ a finite measure, a unitary

operator $U: \mathscr{H} \to L^2(M, d\mu)$, and a real-valued function f on M which is finite a.e. so that

(a) $\psi \in D(A)$ if and only if $f(\cdot)(U\psi)(\cdot) \in L^2(M, d\mu)$.
(b) If $\varphi \in U[D(A)]$, then $(UAU^{-1}\varphi)(m) = f(m)\varphi(m)$.

Proof In the proof of Theorem VIII.3 it was shown that $A + i$ and $A - i$ are one to one and $\mathrm{Ran}(A \pm i) = \mathscr{H}$. Since $A \pm i$ are closed, $(A \pm i)^{-1}$ are closed and therefore bounded (Theorem III.12). By Theorem VIII.2, $(A + i)^{-1}$ and $(A - i)^{-1}$ commute. The equality

$$((A - i)\psi, (A + i)^{-1}(A + i)\varphi) = ((A - i)^{-1}(A - i)\psi, (A + i)\varphi)$$

and the fact that $\mathrm{Ran}(A \pm i) = \mathscr{H}$ shows that $((A + i)^{-1})^* = (A - i)^{-1}$. Thus $(A + i)^{-1}$ is normal.

We now use the easy extension of the spectral theorem for bounded self-adjoint operators to bounded normal operators. The proof of this extension is outlined in Problems 3, 4, and 5 of Chapter VII. We conclude that there is a measure space $\langle M, \mu \rangle$ with μ a finite measure, a unitary operator $U: \mathscr{H} \to L^2(M, \mu)$, and a measurable, bounded, complex-valued function $g(m)$ so that $U(A + i)^{-1}U^{-1}\varphi(m) = g(m)\varphi(m)$ for all $\varphi \in L^2(M, d\mu)$.

Since $\mathrm{Ker}(A + i)^{-1}$ is empty, $g(m) \neq 0$ a.e.$[\mu]$, so the function $f(m) = g(m)^{-1} - i$ is finite a.e.$[\mu]$. Now, suppose $\psi \in D(A)$. Then $\psi = (A + i)^{-1}\varphi$ for some $\varphi \in \mathscr{H}$ and $U\psi = gU\varphi$. Since fg is bounded, we conclude that $f(U\psi) \in L^2(M, d\mu)$. Conversely, if $f(U\psi) \in L^2(M, d\mu)$, then there is a $\varphi \in \mathscr{H}$ so that $U\varphi = (f + i)U\psi$. Thus, $gU\varphi = g(f + i)U\psi = U\psi$, so $\psi = (A + i)^{-1}\varphi$, which shows that $\psi \in D(A)$. This proves (a).

To prove (b) notice that if $\psi \in D(A)$, then $\psi = (A + i)^{-1}\varphi$ for some $\varphi \in \mathscr{H}$ and $A\psi = \varphi - i\psi$. Therefore,

$$\begin{aligned}(UA\psi)(m) &= (U\varphi)(m) - i(U\psi)(m) \\ &= (g(m)^{-1} - i)(U\psi)(m) \\ &= f(m)(U\psi)(m)\end{aligned}$$

Finally, if $\mathrm{Im}(f) > 0$ on a set of nonzero measure, there is a bounded set B in the upper half plane so that $S = \{x \mid f(x) \in B\}$ has nonzero measure. If χ is the characteristic function of S, then $f\chi \in L^2(M, d\mu)$ and $\mathrm{Im}(\chi, f\chi) > 0$. This contradicts the fact that multiplication by f is self-adjoint (since it is unitarily equivalent to A). Thus f is real-valued. ∎

There is a natural way to define functions of a self-adjoint operator by using the above theorem. Given a bounded Borel function h on $\mathbb{R}$ we define

$$h(A) = U^{-1}T_{h(f)}U$$

where $T_{h(f)}$ is the operator on $L^2(M, d\mu)$ which acts by multiplication by the function $h(f(m))$. Using this definition the following theorem follows easily from Theorem VIII.4.

Theorem VIII. 5 (spectral theorem—functional calculus form) Let A be a self-adjoint operator on $\mathscr{H}$. Then there is a unique map $\hat{\phi}$ from the bounded Borel functions on $\mathbb{R}$ into $\mathscr{L}(\mathscr{H})$ so that

(a) $\hat{\phi}$ is an algebraic $*$-homomorphism.
(b) $\hat{\phi}$ is norm continuous, that is, $\|\hat{\phi}(h)\|_{\mathscr{L}(\mathscr{H})} \leq \|h\|_\infty$.
(c) Let $h_n(x)$ be a sequence of bounded Borel functions with $h_n(x) \xrightarrow[n\to\infty]{} x$ for each x and $|h_n(x)| \leq |x|$ for all x and n. Then, for any $\psi \in D(A)$, $\lim_{n\to\infty} \hat{\phi}(h_n)\psi = A\psi$.
(d) If $h_n(x) \to h(x)$ pointwise and if the sequence $\|h_n\|_\infty$ is bounded, then $\hat{\phi}(h_n) \to \hat{\phi}(h)$ strongly.

In addition:

(e) If $A\psi = \lambda\psi$, $\hat{\phi}(h)\psi = h(\lambda)\psi$.
(f) If $h \geq 0$, then $\hat{\phi}(h) \geq 0$.

The functional calculus is very useful. For example, it allows us to define the exponential e^{itA} and prove easily many of its properties as a function of t (see the next section). In the case where A is bounded we do not need the functional calculus to define the exponential since we can define e^{itA} by the power series which converges in norm.

The functional calculus is also used to construct spectral measures and can be used to develop a multiplicity theory similar to that for bounded self-adjoint operators. A vector ψ is said to be **cyclic** for A if $\{g(A)\psi \mid g \in C_\infty(\mathbb{R})\}$ is dense in $\mathscr{H}$. If ψ is a cyclic vector, then it is possible to represent $\mathscr{H}$ as $L^2(\mathbb{R}, d\mu_\psi)$ where μ_ψ is the measure satisfying

$$\int_{\mathbb{R}} g(x)\, d\mu_\psi(x) = (\psi, g(A)\psi)$$

in such a way that A becomes multiplication by x. In general, $\mathscr{H}$ decomposes into a direct sum of cyclic subspaces so the measure space, M, in Theorem VIII.4 can be realized as a union of copies of $\mathbb{R}$. As in the case of bounded operators we can define $\sigma_{ac}(A)$, $\sigma_{pp}(A)$, $\sigma_{sing}(A)$, and decompose $\mathscr{H}$ accordingly.

Finally, the spectral theorem in its projection-valued measure form follows easily from the functional calculus. Let P_Ω be the operator $\chi_\Omega(A)$ where χ_Ω is the characteristic function of the measurable set $\Omega \subset \mathbb{R}$. The family of operators $\{P_\Omega\}$ has the following properties:

(a) Each P_Ω is an orthogonal projection.
(b) $P_\varnothing = 0$, $P_{(-\infty,\infty)} = I$
(c) If $\Omega = \bigcup_{n=1} \Omega_n$ with $\Omega_n \cap \Omega_m = \varnothing$ if $n \neq m$, then $P_\Omega = \text{s-lim}_{N\to\infty} \sum_{n=1}^{N} P_{\Omega_n}$
(d) $P_{\Omega_1} P_{\Omega_2} = P_{\Omega_1 \cap \Omega_2}$

Such a family is called a **projection-valued measure** (p.v.m.). This is a generalization of the notion of bounded projection-valued measure introduced in Chapter VII in that we only require $P_{(-\infty,\infty)} = I$ rather than $P_{(-a,a)} = I$ for some a. For $\varphi \in \mathscr{H}$, $(\varphi, P_\Omega \varphi)$ is a well-defined Borel measure on $\mathbb{R}$ which we denote by $d(\varphi, P_\lambda \varphi)$ as in Chapter VII. The complex measure $d(\varphi, P_\lambda \psi)$ is defined by polarization. Thus, given a bounded Borel function g we can define $g(A)$ by

$$(\varphi, g(A)\varphi) = \int_{-\infty}^{\infty} g(\lambda)\, d(\varphi, P_\lambda \varphi) \tag{VIII.4}$$

It is not difficult to show that this map $g \mapsto g(A)$ has the properties (a)–(d) of Theorem VIII.5, so $g(A)$ as defined by (VIII.4) coincides with the definition of $g(A)$ given by Theorem VIII.4. Now, suppose g is an unbounded complex-valued Borel function and let

$$D_g = \{\varphi \mid \int_{-\infty}^{\infty} |g(\lambda)|^2\, d(\varphi, P_\lambda \varphi) < \infty\} \tag{VIII.5}$$

Then, D_g is dense in $\mathscr{H}$ and an operator $g(A)$ is defined on D_g by

$$(\varphi, g(A)\varphi) = \int_{-\infty}^{\infty} g(\lambda)\, d(\varphi, P_\lambda \varphi)$$

As in Chapter VII, we write symbolically

$$g(A) = \int g(\lambda)\, dP_\lambda$$

In particular, for $\varphi, \psi \in D(A)$,

$$(\varphi, A\psi) = \int_{-\infty}^{\infty} \lambda\, d(\varphi, P_\lambda \psi)$$

If g is real-valued, then $g(A)$ is self-adjoint on D_g. We summarize:

Theorem VIII.6 (spectral theorem—projection valued measure form) There is a one-to-one correspondence between self-adjoint operators A and projection-valued measures $\{P_\Omega\}$ on $\mathscr{H}$, the correspondence being given by

$$A = \int_{-\infty}^{\infty} \lambda\, dP_\lambda$$

Definition If $U(t)$ is a strongly continuous one-parameter unitary group, then the self-adjoint operator A with $U(t) = e^{itA}$ is called the **infinitesimal generator** of $U(t)$.

Suppose that $U(t)$ is a *weakly* continuous one-parameter unitary group. Then

$$\| U(t)\varphi - \varphi \|^2 = \| U(t)\varphi \|^2 - (U(t)\varphi, \varphi) - (\varphi, U(t)\varphi) + \| \varphi \|^2$$
$$\to 2\| \varphi \|^2 - 2\| \varphi \|^2 = 0$$

as $t \to 0$. Thus $U(t)$ is actually *strongly* continuous. As a matter of fact, to conclude that $U(t)$ is strongly continuous one need only show that $U(t)$ is weakly measurable, that is, that $(U(t)\varphi, \psi)$ is measurable for each φ and ψ. This startling result, proven by von Neumann, is sometimes useful since in applications one can often show that $(U(t)\varphi, \psi)$ is the limit of a sequence of continuous functions; $(U(t)\varphi, \psi)$ is therefore measurable and by von Neumann's theorem $U(t)$ is then strongly continuous.

Theorem VIII.9 (von Neumann) Let $U(t)$ be a one-parameter group of unitary operators on a *separable* Hilbert space $\mathscr{H}$. Suppose that for all φ, $\psi \in \mathscr{H}$, $(U(t)\psi, \varphi)$ is measurable. Then $U(t)$ is strongly continuous.

Proof Let $\psi \in \mathscr{H}$. Then for all $\varphi \in \mathscr{H}$, $(U(t)\psi, \varphi)$ is a bounded measurable function and

$$\varphi \mapsto \int_0^a (U(t)\psi, \varphi)\, dt$$

is a linear functional on $\mathscr{H}$ of norm less than or equal to $a\|\psi\|$. Thus, by the Riesz lemma there is a $\psi_a \in \mathscr{H}$ so that

$$(\psi_a, \varphi) = \int_0^a (U(t)\psi, \varphi)\, dt$$

Now,

$$(U(b)\psi_a, \varphi) = (\psi_a, U(-b)\varphi)$$
$$= \int_0^a (U(t)\psi, U(-b)\varphi)\, dt$$
$$= \int_0^a (U(t+b)\psi, \varphi)\, dt$$
$$= \int_b^{a+b} (U(t)\psi, \varphi)\, dt$$

Thus

$$|(U(b)\psi_a, \varphi) - (\psi_a, \varphi)| = \left|\int_0^b (U(t)\psi, \varphi)\, dt\right| + \left|\int_a^{a+b} (U(t)\psi, \varphi)\, dt\right|$$
$$\leq 2b\|\varphi\|\,\|\psi\|$$

Therefore,

$$\lim_{b\to 0} (U(b)\psi_a, \varphi) = (\psi_a, \varphi)$$

so that $U(b)$ is weakly and therefore strongly continuous on the set of vectors of the form $\{\psi_a | \psi \in \mathscr{H}\}$. It remains only to show that this set is dense, since by by an $\varepsilon/3$ argument we can then conclude that $t \mapsto U(t)$ is strongly continuous on $\mathscr{H}$. Suppose that $\varphi \in \{\psi_a | \psi \in \mathscr{H}, a \in \mathbb{R}\}^\perp$ and let $\{\psi^{(n)}\}$ be an orthonormal basis for $\mathscr{H}$. Then for each n,

$$0 = (\psi_a^{(n)}, \varphi) = \int_0^a (U(t)\psi^{(n)}, \varphi)\, dt$$

for all a which implies that $(U(t)\psi^{(n)}, \varphi) = 0$ except for $t \in S_n$, a set of measure zero. Choose $t_0 \notin \bigcup_{n=1}^\infty S_n$. Then $(U(t_0)\psi^{(n)}, \varphi) = 0$ for all n which implies that $\varphi = 0$, since $U(t_0)$ is unitary. ∎

The proof of essential self-adjointness in Theorem VIII.8 directly implies the following self-adjointness criterion.

Theorem VIII.10 Suppose that $U(t)$ is a strongly continuous one-parameter unitary group. Let D be a dense domain which is invariant under $U(t)$ and on which $U(t)$ is strongly differentiable. Then i^{-1} times the strong derivative of $U(t)$ is essentially self-adjoint on D and its closure is the infinitesimal generator of $U(t)$.

This theorem has a reformulation which is sufficiently important that we state it as a theorem.

Theorem VIII.11 Let A be a self-adjoint operator on $\mathscr{H}$ and D be a dense linear set contained in $D(A)$. If for all t, e^{itA}: $D \to D$, then D is a core for A.

Finally, we have the following generalization of Stone's theorem.

If $g(\cdot)$ is a real-valued Borel function on $\mathbb{R}$, then

$$g(A) = \int_{-\infty}^{\infty} g(\lambda)\, dP_\lambda$$

defined on D_g (VIII.5) is self-adjoint. If g is bounded, $g(A)$ coincides with $\hat{\phi}(g)$ in Theorem VIII.5.

We conclude with several remarks. First, Stone's formula, given in Theorem VII.13, relates the resolvent and the projection-valued measure associated with any self-adjoint operator. The proof is the same as in the bounded case.

The spectrum of an unbounded self-adjoint operator is an unbounded subset of the real axis. One can define discrete and essential spectrum; they are still characterized by Theorems VII.9, VII.10, and VII.11. Theorem VII.12 (Weyl's criterion) still holds if one adds the criterion that the vectors $\{\psi_n\}$ must be in the domain of A.

Finally, we note that the measure space of Theorem VIII.4 can always be chosen so that Proposition 2 is applicable:

Proposition 3 Let A be a self-adjoint operator on a separable Hilbert space $\mathscr{H}$. Then the measure space $\langle M, \mu\rangle$ and the function f of Theorem VIII.4 can be chosen so that $f \in L^p(M, d\mu)$ for all p with $1 \leq p < \infty$.

Proof By Theorem VIII.4, we know that A is unitarily equivalent to T_f on some measure space $\langle M, \nu\rangle$ with $\nu(M) < \infty$. Let μ be the measure given by

$$d\mu = e^{-f^2}\, d\nu$$

Then T_f on $L^2(M, d\mu)$ is unitarily equivalent to T_f on $L^2(M, d\nu)$ under $V: L^2(M, d\nu) \to L^2(M, d\mu)$ given by $Vg(m) = (e^{+f^2/2}g)(m)$. Moreover, $f \in L^p(M, d\mu)$ for any $1 \leq p < \infty$. ∎

VIII.4 Stone's theorem

In this section we prove a theorem due to Stone which, like the spectral theorem, is fundamental for quantum mechanics. Suppose that A is a self-adjoint operator on $\mathscr{H}$. If A is bounded, we can define the exponential of A by

$$e^{itA} = \sum_{n=0}^{\infty} \frac{(it)^n A^n}{n!}$$

since the series converges in norm. If A unbounded *and* self-adjoint, we cannot use the power series directly, but we can use the functional calculus developed in the last section to define e^{itA}.

Theorem VIII.7 Let A be a self-adjoint operator and define $U(t) = e^{itA}$. Then

(a) For each $t \in \mathbb{R}$, $U(t)$ is a unitary operator and $U(t+s) = U(t)U(s)$ for all $s, t \in \mathbb{R}$.

(b) If $\varphi \in \mathscr{H}$ and $t \to t_0$, then $U(t)\varphi \longrightarrow U(t_0)\varphi$.

(c) For $\psi \in D(A)$, $\dfrac{U(t)\psi - \psi}{t} \longrightarrow iA\psi$ as $t \to 0$.

(d) If $\lim\limits_{t\to 0} \dfrac{U(t)\psi - \psi}{t}$ exists, then $\psi \in D(A)$.

Proof (a) follows immediately from the functional calculus and the corresponding statements for the complex-valued function $e^{it\lambda}$. To prove (b) observe that

$$\|e^{itA}\varphi - \varphi\|^2 = \int_R |e^{it\lambda} - 1|^2 \, d(P_\lambda \varphi, \varphi)$$

Since $|e^{it\lambda} - 1|^2$ is dominated by the integrable function $g(\lambda) = 2$ and since

$$|e^{it\lambda} - 1|^2 \xrightarrow[t\to 0]{} 0 \qquad \text{for each } \lambda \in \mathbb{R}$$

we conclude that $\|U(t)\varphi - \varphi\|^2 \to 0$ by the Lebesgue dominated-convergence theorem. Thus $t \mapsto U(t)$ is strongly continuous at $t = 0$, which by the group property proves $t \mapsto U(t)$ is strongly continuous everywhere. The proof of (c), which again uses the dominated convergence theorem and the estimate $|e^{ix} - 1| \leq |x|$, is left to the reader (Problem 11). To prove (d), we define

$$D(B) = \{\psi \mid \lim_{t\to 0} \frac{U(t)\psi - \psi}{t} \text{ exists}\}$$

and let $iB\psi = \lim_{t\to 0} [U(t)\psi - \psi]/t$. A simple computation shows that B is symmetric. By (c), $B \supset A$, so $B = A$. ∎

Definition An operator-valued function $U(t)$ satisfying (a) and (b) is called **a strongly continuous one-parameter unitary group.**

The following theorem says that every strongly continuous unitary group arises as the exponential of a self-adjoint operator.

Theorem VIII.12 Let $t \to U(t) = U(t_1, \ldots, t_n)$ be a strongly continuous map of $\mathbb{R}^n$ into the unitary operators on a separable Hilbert space $\mathscr{H}$ satisfying $U(t + s) = U(t)U(s)$ and $U(0) = I$. Let D be the set of finite linear combinations of vectors of the form

$$\varphi_f = \int_{\mathbb{R}^n} f(t)U(t)\varphi \, dt \qquad \varphi \in \mathscr{H}, \quad f \in C_0^\infty(\mathbb{R}^n)$$

Then D is a domain of essential self-adjointness for each of the generators A_j of the one-parameter subgroups $U(0, 0, \ldots, t_j, \ldots, 0)$, each A_j: $D \to D$ and the A_j commute, $j = 1, \ldots, n$. Furthermore, there is a projection-valued measure P_Ω on $\mathbb{R}^n$ so that

$$(\varphi, U(t)\,\psi) = \int_{\mathbb{R}^n} e^{it\cdot\lambda} d(\varphi, P_\lambda \psi)$$

for all $\varphi, \psi \in \mathscr{H}$.

Proof Let A_j be the infinitesimal generator of $U_j(t_j) = U(0, \ldots, t_j, \ldots, 0)$. The procedure used in the proof of Theorem VIII.8 shows that $D \subset D(A_j)$, A_j: $D \to D$, and $U_j(t_j)$: $D \to D$. Theorem VIII.11 shows that A_j is essentially self-adjoint on D. Because of the relation $U(t + s) = U(t)U(s)$, $U_j(t_j)$ commutes with $U_i(t_i)$ for all t_i, $t_j \in \mathbb{R}$. Therefore, it follows from Theorem VIII.13, that A_i and A_j commute in the sense defined in the next section; that is, their spectral projections commute.

Let P_Ω^j be the projection-valued measure on $\mathbb{R}$ corresponding to A_j. Define a projection valued measure P_Ω on $\mathbb{R}^n$ by defining it first on rectangles $r = (a_1, b_1) \times \cdots \times (a_n, b_n)$ by $P_r = P^1_{(a_1,b_1)} P^2_{(a_2,b_2)} \cdots P^n_{(a_n,b_n)}$ and then letting P_Ω be the unique extension to the smallest σ-algebra containing the rectangles, namely the Borel sets. Notice that, by Theorem VIII.13, the $P^j_{\Omega_j}$ commute since the groups U_j commute. For each $\varphi, \psi \in \mathscr{H}$, $(\varphi, P_\Omega \psi)$ is a complex-valued measure of finite mass which we denote by $d(\varphi, P_\lambda \psi)$. Applying Fubini's theorem we easily conclude that

$$\begin{aligned}\int_{\mathbb{R}^n} e^{it\cdot\lambda}\, d(\varphi, P_\lambda \psi) &= (\varphi, U_1(t_1) \ldots, U_n(t_n)\psi) \\ &= (\varphi, U(t)\psi) \quad \blacksquare\end{aligned}$$

VIII.5 Formal manipulation is a touchy business: Nelson's example

From the theorems proven in the last two sections it may seem to the reader that unbounded operators are just like bounded operators except that one needs to be a little careful about domains. First, of all, it is sometimes

difficult to determine the domain of a self-adjoint operator exactly, and it is not always enough to check statements on a core. Furthermore, formal calculations can be misleading. These statements are illustrated by the question of commutativity and the surprising example of Nelson which show how difficult it is to deal with unbounded operators.

Suppose that A and B are two unbounded self-adjoint operators on a Hilbert space $\mathscr{H}$. We would like to find a reasonable meaning for the statement "A and B commute." This cannot be done in the straightforward way since $AB - BA$ may not make sense on any vector in $\mathscr{H}$; for example, one might have $(\text{Ran } A) \cap D(B) = \{0\}$ in which case BA does not have a meaning. This suggests that we find an equivalent formulation of commutativity for bounded self-adjoint operators. The spectral theorem for bounded self-adjoint operators A and B shows that in that case $AB - BA = 0$ if and only if all their projections, $\{P_\Omega^A\}$ and $\{P_\Omega^B\}$, commute. We take this as our definition in the unbounded case.

Definition Two (possibly unbounded) self-adjoint operators A and B are said to **commute** if and only if all the projections in their associated projection-valued measures commute.

The spectral theorem shows that if A and B commute, then all the bounded Borel functions of A and B also commute. In particular, the resolvents $R_\lambda(A)$ and $R_\mu(B)$ commute and the unitary groups e^{itA} and e^{isB} commute. The converse statement is also true and this shows that the above definition of "commute" is reasonable:

Theorem VIII.13 Let A and B be self-adjoint operators on a Hilbert space $\mathscr{H}$. Then the following three statements are equivalent:

(a) A and B commute.
(b) If $\text{Im } \lambda$ and $\text{Im } \mu$ are nonzero, then $R_\lambda(A)R_\mu(B) = R_\mu(B)R_\lambda(A)$.
(c) For all $s, t \in \mathbb{R}$, $e^{itA}e^{isB} = e^{isB}e^{itA}$.

Proof The fact that (a) implies (b) and (c) follows from the functional calculus. The fact that (b) implies (a) easily follows from the formula which expresses the spectral projections of A and B as strong limits of the resolvents (Stone's formula) together with the fact that

$$\text{s-lim}_{\varepsilon \downarrow 0} i\varepsilon R_{a+i\varepsilon}(A) = P_{\{a\}}^A$$

To prove that (c) implies (a), we use some simple facts about the Fourier

Theorem VIII.8 (Stone's theorem) Let $U(t)$ be a strongly continuous one-parameter unitary group on a Hilbert space $\mathscr{H}$. Then, there is a self-adjoint operator A on $\mathscr{H}$ so that $U(t) = e^{itA}$.

Proof Part (d) of Theorem VIII.7 suggests that we obtain A by differentiating $U(t)$ at $t = 0$. We will show that this can be done on a dense set of especially nice vectors and then show that the limiting operator is essentially self-adjoint by using the basic criterion. Finally, we show that the exponential of this limiting operator is just $U(t)$.

Let $f \in C_0^\infty(\mathbb{R})$ and for each $\varphi \in \mathscr{H}$ define

$$\varphi_f = \int_{-\infty}^{\infty} f(t)U(t)\varphi \, dt$$

Since $U(t)$ is strongly continuous the integral can be taken to be a Riemann integral. Let D be the set of finite linear combinations of all such φ_f for $\varphi \in \mathscr{H}$ and $f \in C_0^\infty(\mathbb{R})$. If $j_\varepsilon(x)$ is the approximate identity introduced in Section VIII.1, then

$$\begin{aligned} \|\varphi_{j_\varepsilon} - \varphi\| &= \left\| \int_{-\infty}^{\infty} j_\varepsilon(t)(U(t)\varphi - \varphi)\, dt \right\| \\ &\leq \left(\int_{-\infty}^{\infty} j_\varepsilon(t)\, dt \right) \sup_{t \in [-\varepsilon, \varepsilon]} \|U(t)\varphi - \varphi\| \end{aligned}$$

Since $U(t)$ is strongly continuous, D is dense in $\mathscr{H}$. We have used the inequality $\|\int h(t)\, dt\| \leq \int \|h(t)\|\, dt$ for Banach space-valued continuous functions on the real line (which can be proven using the approximate partial sums as in the real-valued case).

For $\varphi_f \in D$, we compute

$$\begin{aligned} \left(\frac{U(s) - I}{s}\right)\varphi_f &= \int_{-\infty}^{\infty} f(t)\left(\frac{U(s+t) - U(t)}{s}\right)\varphi \, dt \\ &= \int_{-\infty}^{\infty} \frac{f(\tau - s) - f(\tau)}{s} U(\tau)\varphi \, d\tau \\ &\to -\int f'(\tau)U(\tau)\varphi \, d\tau \\ &= \varphi_{-f'} \end{aligned}$$

since $[f(\tau - s) - f(\tau)]/s$ converges to $-f'(\tau)$ uniformly. For $\varphi_f \in D$, we define $A\varphi_f = i^{-1}\varphi_{-f'}$. Notice that $U(t)\colon D \to D$, $A\colon D \to D$, and $U(t)A\varphi_f =$

$AU(t)\varphi_f$ for $\varphi_f \in D$. Furthermore, if $\varphi_f, \varphi_g \in D$, we have

$$\begin{aligned}(A\varphi_f, \varphi_g) &= \lim_{s\to 0}\left(\left(\frac{U(s)-I}{is}\right)\varphi_f, \varphi_g\right)\\ &= \lim_{s\to 0}\left(\varphi_f, \left(\frac{I-U(-s)}{is}\right)\varphi_g\right)\\ &= \left(\varphi_f, \frac{1}{i}\varphi_{-g'}\right)\\ &= (\varphi_f, A\varphi_g)\end{aligned}$$

so A is symmetric.

Now we show that A is essentially self-adjoint. Suppose that there is a $u \in D(A^*)$ so that $A^*u = iu$. Then for each $\varphi \in D(A) = D$,

$$\begin{aligned}\frac{d}{dt}(U(t)\varphi, u) &= (iAU(t)\varphi, u)\\ &= -i(U(t)\varphi, A^*u)\\ &= -i(U(t)\varphi, iu)\\ &= (U(t)\varphi, u)\end{aligned}$$

Thus, the complex-valued function $f(t) = (U(t)\varphi, u)$ satisfies the ordinary differential equation $f' = f$ so $f(t) = f(0)e^t$. Since $U(t)$ has norm one, $|f(t)|$ is bounded, which implies that $f(0) = (\varphi, u) = 0$. Since D is dense, $u = 0$. A similar proof shows that $A^*u = -iu$ can have no nonzero solutions. Therefore, by the corollary to Theorem VIII.3, A is essentially self-adjoint on D.

Let $V(t) = e^{it\bar{A}}$. It remains to show that $U(t) = V(t)$. Let $\varphi \in D$. Since $\varphi \in D(\bar{A})$, $V(t)\varphi \in D(\bar{A})$ and $V'(t)\varphi = iAV(t)\varphi$ by (c) of Theorem VIII.7. We already know that $U(t)\varphi \in D \subset D(\bar{A})$ for all t. Let $w(t) = U(t)\varphi - V(t)\varphi$. Then $w(t)$ is a strongly differentiable vector-valued function and

$$\begin{aligned}w'(t) &= iAU(t)\varphi - i\bar{A}V(t)\varphi\\ &= i\bar{A}w(t)\end{aligned}$$

Thus

$$\begin{aligned}\frac{d}{dt}\|w(t)\|^2 &= -i(\bar{A}w(t), w(t)) + i(w(t), \bar{A}w(t))\\ &= 0\end{aligned}$$

Therefore $w(t) = 0$ for all t since $w(0) = 0$. This implies that $U(t)\varphi = V(t)\varphi$ for all $t \in \mathbb{R}$, $\varphi \in D$. Since D is dense, $U(t) = V(t)$. ∎

transform proven in Section IX.1. Let $f \in \mathscr{S}(\mathbb{R})$. Then, by Fubini's theorem,

$$\begin{aligned}\int_{-\infty}^{\infty} f(t)(e^{itA}\varphi, \psi)\, dt &= \int_{-\infty}^{\infty} f(t)\left(\int_{-\infty}^{\infty} e^{-it\lambda} d_\lambda(P_\lambda^A \varphi, \psi)\right) dt \\ &= \sqrt{2\pi} \int_{-\infty}^{\infty} \hat{f}(\lambda)\, d_\lambda(P_\lambda^A \varphi, \psi) \\ &= \sqrt{2\pi}(\varphi, \hat{f}(A)\psi)\end{aligned}$$

Thus, using (c) and Fubini's theorem again,

$$\begin{aligned}(\varphi, \hat{f}(A)\hat{g}(B)\psi) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(t)g(s)(\varphi, e^{-itA}e^{-isB}\psi)\, ds\, dt \\ &= (\varphi, \hat{g}(B)\hat{f}(A)\psi)\end{aligned}$$

so, for all $f, g \in \mathscr{S}(\mathbb{R})$, $\hat{f}(A)\hat{g}(B) - \hat{g}(B)\hat{f}(A) = 0$. Since the Fourier transform maps $\mathscr{S}(\mathbb{R})$ onto $\mathscr{S}(\mathbb{R})$ we conclude that $f(A)g(B) = g(B)f(A)$ for all $f, g \in \mathscr{S}(\mathbb{R})$. But, the characteristic function, $\chi_{(a,b)}$ can be expressed as the pointwise limit of a sequence f_n of uniformly bounded functions in $\mathscr{S}$. By the functional calculus,

$$f_n(A) \xrightarrow{s} P^A_{(a,b)}$$

Similarly, we find uniformly bounded $g_n \in A$ converging pointwise to $\chi_{(c,d)}$ and

$$g_n(B) \xrightarrow{s} P^B_{(c,d)}$$

Since the f_n and g_n are uniformly bounded and

$$f_n(A)g_n(B) = g_n(B)f_n(A)$$

for each n, we conclude that $P^A_{(a,b)}$ and $P^B_{(c,d)}$ commute which proves (a). ∎

Although the above theorem shows that the definition of "commute" is reasonable, it is not always easy to deal with. In practice, one is usually given A and B on sets of essential self-adjointness, $D_0(A)$ and $D_0(B)$, and it may be very difficult to construct the spectral projections, the resolvents, or the groups corresponding to $\bar{A}$ and $\bar{B}$. Thus, one would like to have a criterion in terms of the operators themselves. In Problem 13, the reader is asked to find disjoint domains of essential self-adjointness for the operators x and x^2 on $L^2(\mathbb{R})$, so such a commutativity criterion could never be necessary, but with enough restrictions might be sufficient. Here are two conjectures which seem reasonable but which are *false*:

1. Let D be a dense subspace in $\mathscr{H}$ which is contained in the domains of A and B. Suppose further that $A: D \to D$ and $B: D \to D$. Then, if $AB\varphi - BA\varphi = 0$ for each $\varphi \in D$, A and B commute (*FALSE*!).

2. Let D be a dense domain of essential self-adjointness for A and B. Suppose further that $A: D \to D$ and $B: D \to D$. Then, if $ABφ - BAφ = 0$ for all $φ \in D$, A commutes with B (*FALSE*!).

Both of these statements are *false*, the hypotheses are *not* sufficient to guarantee commutativity. This is surprising for several reasons. First, the conditions seem reasonable. Secondly, in condition (2), D is assumed to be a domain of essential self-adjointness for both A and B, so the action of A and B on D should provide enough information to determine whether A and B commute. Finally, in a formal sense

$$e^{itA} \approx I + \sum_{n=1}^{\infty} \frac{(itA)^n}{n!}$$
$$e^{isB} \approx I + \sum_{n=1}^{\infty} \frac{(isB)^n}{n!} \tag{VIII.6}$$

Since it follows from the conditions in (1) and (2) that $A^nB^mφ - B^mA^nφ = 0$ for all $φ \in D$, one might expect that e^{itA} and e^{isB} commute for all s and t. By Theorem VIII.13 this would imply that A and B commute. The trouble with this argument is that the expressions in (VIII.6) are only formal and may have meaning on no vectors in D since A and B are unbounded. The finite sums make sense on D and

$$\left(I + \sum_{n=1}^{N} \frac{(itA)^n}{n!}\right)\left(I + \sum_{m=1}^{M} \frac{(isB)^m}{m!}\right)φ = \left(I + \sum_{m=1}^{M} \frac{(isB)^m}{m!}\right)\left(I + \sum_{n=1}^{N} \frac{(itA)^n}{n!}\right)φ$$

but we cannot conclude from this that e^{itA} and e^{isB} commute. The following example is due to Nelson.

Example 1 Suppose that M is the Riemann surface of the $\sqrt{z}$ and $\mathscr{H} = L^2(M)$ with Lebesgue measure (locally). Let $A = -i\partial/\partial x$ and $B = -i\partial/\partial y$ on the domain D which consists of all infinitely differentiable functions with compact support not containing the origin. Then

(a) A and B are essentially self-adjoint on D.
(b) $A: D \to D$, $B: D \to D$
(c) $ABφ = BAφ$ for $φ \in D$
(d) e^{itA} and e^{isB} do not commute.

The proofs of (b) and (c) are obvious. To prove (a), first observe that integration by parts shows that A and B are symmetric. Let $D_x \subset D$ be the functions in D whose support does not contain the x axis on either sheet. D_x is also dense in $L^2(M)$. On D_x define $(U(t)φ)(x, y) = φ(x + t, y)$. Then $U(t)$ is a norm-preserving map with dense range and so extends to a unitary operator on

$L^2(M)$. Since $U(t)$ is strongly continuous on D_x, $U(t)$ is strongly continuous on $L^2(M)$. Now, on D_x, $U(t)$ is strongly differentiable and i^{-1} times its strong derivative is A. Thus, by Theorem VIII.10, A is essentially self-adjoint on D_x and therefore on D (Problem 14) and its closure generates $U(t)$. A similar proof shows that the closure of B is the infinitesimal generator of translation in the y direction defined by extension from a domain D_y. This proves (a).

To prove (d), let φ be an infinitely differentiable function with support contained in a small circle about the point $(-\frac{1}{2}, -\frac{1}{2})$ on the first sheet. Then

$$U(1)V(1)\varphi \neq V(1)U(1)\varphi$$

since the functions will have their support around $(\frac{1}{2}, \frac{1}{2})$ on different sheets. ∎

Example 2 (canonical commutation relations) A pair P, Q of self-adjoint operators is said to "satisfy" the **canonical commutation relations** if

$$PQ - QP = -iI \tag{VIII.7}$$

P and Q cannot both be bounded. For, if they were, the relation $PQ^n - Q^nP = -inQ^{n-1}$ [which follows directly from (VIII.7)] would imply

$$n\|Q\|^{n-1} = n\|Q^{n-1}\| \leq 2\|P\|\,\|Q\|^n$$

So for all n, $2\|P\|\,\|Q\| \geq n$, which is a contradiction. Thus, either P or Q or both must be unbounded so we cannot discuss the relation (VIII.7) without worrying about domains. The standard realization or "representation" used in quantum mechanics is the **Schrödinger representation** where $\mathscr{H} = L^2(\mathbb{R})$ and P and Q are the closures of $i^{-1}d/dx$ and multiplication by x on $\mathscr{S}(\mathbb{R})$. $\mathscr{S}(\mathbb{R})$ is a domain of essential self-adjointness for $i^{-1}d/dx$ and x,

$$\frac{1}{i}\frac{d}{dx} : \mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R}), \qquad x : \mathscr{S}(\mathbb{R}) \to \mathscr{S}(\mathbb{R})$$

and for $\varphi \in \mathscr{S}(\mathbb{R})$,

$$\frac{1}{i}\frac{d}{dx}(x\varphi) - x\left(\frac{1}{i}\frac{d}{dx}\varphi\right) = -i\varphi$$

The question is: in what sense is the Schrödinger representation the "only" representation of the relation (VIII.7). One method of dealing with (VIII.7) is with the unitary groups. If $U(t) = e^{itP}$ and $V(s) = e^{isQ}$, then a *formal* calculation using (VIII.7) and the formal power series expansion for e^{itP} and e^{isQ} yields

$$U(t)V(s) = e^{its}V(s)U(t) \tag{VIII.8}$$

The reader should not be surprised to learn that the two problems, solving the relation (VIII.7) and solving the relation (VIII.8), which are related by a formal calculation are *not* equivalent. Let us first discuss (VIII.8), which is an easier problem because we need deal only with bounded operators. Two continuous one-parameter groups satisfying (VIII.8) are said to satisfy the **Weyl relations**. The reader can easily check that in the Schrödinger representation, the groups e^{itP} and e^{isQ} *do* satisfy the Weyl relations; e^{itP} is just translation to the left by t, and e^{isQ} is multiplication by e^{isx}. The following theorem states that up to multiplicity and unitary equivalence, the Weyl relations have only one solution (for a proof see Theorem XI.84 or Problem 30 in Chapter X).

Theorem VIII.14 (von Neumann) Let $U(t)$ and $V(s)$ be one-parameter, continuous, unitary groups on a separable Hilbert space $\mathscr{H}$ satisfying the Weyl relations. Then, there are closed subspaces $\mathscr{H}_\ell$ so that

(a) $\mathscr{H} = \oplus_{\ell=1}^{N} \mathscr{H}_\ell$ (N a positive integer or ∞)
(b) $U(t)\colon \mathscr{H}_\ell \to \mathscr{H}_\ell$, $V(s)\colon \mathscr{H}_\ell \to \mathscr{H}_\ell$ for all $s, t \in \mathbb{R}$.
(c) For each ℓ, there is a unitary operator $T_\ell\colon \mathscr{H}_\ell \to L^2(\mathbb{R})$ such that $T_\ell U(t) T_\ell^{-1}$ is translation to the left by t and $T_\ell V(s) T_\ell^{-1}$ is multiplication by e^{isx}.

Corollary Let $U(t)$ and $V(s)$ be continuous one-parameter unitary groups satisfying the Weyl relations on a separable Hilbert space $\mathscr{H}$. Let P be the generator of $U(t)$, Q the generator of $V(s)$. Then there is a dense domain $D \subset \mathscr{H}$ so that

(a) $P\colon D \to D$, $Q\colon D \to D$
(b) $PQ\varphi - QP\varphi = -i\varphi$ for all $\varphi \in D$
(c) P and Q are essentially self-adjoint on D.

This corollary (whose easy proof is given as Problem 36) shows that any solution of the Weyl relations has infinitesimal generators which satisfy the canonical commutation relations in the sense given by (a), (b), and (c). The converse of this statement is not true as is shown by the following slight perturbation of Nelson's example. Let $\mathscr{H} = L^2(M)$ as in Example 1,

$$P = \frac{1}{i}\frac{\partial}{\partial x} \qquad Q = x + \frac{1}{i}\frac{\partial}{\partial y}$$

on the domain D given there. P and Q satisfy properties (a), (b), and (c). The proof of self-adjointness is similar to the proof in Example 1. But the groups they generate do not satisfy the Weyl relations.

One point of this section was to show that formal calculations with the formal power series expansion for e^{itA} can lead to false conclusions. This does not imply that one can never make sense out of the formal series for e^{itA} if A is unbounded. In fact, suppose that A is an unbounded self-adjoint operator and P_Ω is the corresponding projection-valued measure. Then the set D_c of vectors of the form $P_{[-M,M]}\varphi$, where $\varphi \in \mathscr{H}$ and M is arbitrary but finite, is a dense set contained in $D(A^n)$ for all n and A is essentially self-adjoint on D_c. Furthermore, if $\psi = P_{[-M,M]}\varphi$, then $\|A^n\psi\| \leq M^n\|\psi\|$, so

$$\sum_{n=0}^{\infty} \frac{t^n\|A^n\psi\|}{n!} < \infty \tag{VIII.9}$$

for all t. Therefore, if $\psi \in D_c$ the series $\sum_{n=0}^{\infty} (it)^n A^n\psi/n!$ converges. Vectors $\psi \in \bigcap_{n=1}^{\infty} D(A^n)$ which satisfy (VIII.9) for some $t > 0$ are called **analytic vectors** for A. On such vectors the power series for $e^{itA}\psi$ makes sense and converges to $e^{itA}\psi$ as long as t is sufficiently small. We will return to analytic vectors in Section X.6 where we prove a theorem of Nelson that if a symmetric operator A has a dense set of analytic vectors in its domain D then A is essentially self-adjoint.

VIII.6 Quadratic forms

One consequence of the Riesz lemma is that there is a one-to-one correspondence between bounded quadratic forms and bounded operators; that is, any sesquilinear map $q: \mathscr{H} \times \mathscr{H} \to \mathbb{C}$ which satisfies $|q(\varphi, \psi)| \leq M\|\varphi\|\,\|\psi\|$ is of the form $q(\varphi, \psi) = (\varphi, A\psi)$ for some bounded operator A. As one might expect, the situation is more complicated if one removes the boundedness restriction. It is the relationship between unbounded forms and unbounded operators which we study briefly in this section.

Definition A **quadratic form** is a map q: $Q(q) \times Q(q) \to \mathbb{C}$, where $Q(q)$ is a dense linear subset of $\mathscr{H}$ called the **form domain**, such that $q(\cdot, \psi)$ is conjugate linear and $q(\varphi, \cdot)$ is linear for $\varphi, \psi \in Q(q)$. If $q(\varphi, \psi) = \overline{q(\psi, \varphi)}$ we say that q is **symmetric**. If $q(\varphi, \varphi) \geq 0$ for all $\varphi \in Q$, q is called **positive**, and if $q(\varphi, \varphi) \geq -M\|\varphi\|^2$ for some M, we say that q is **semibounded**.

Notice that if q is semibounded, then it is automatically symmetric if $\mathscr{H}$ is complex.

Example 1 Let $\mathscr{H} = L^2(\mathbb{R})$ and $Q(q) = C_0^\infty(\mathbb{R})$ with $q(f, g) = \bar{f}(0)g(0)$. Then q is a positive quadratic form. Since $q(f, g) = \delta(\bar{f}g)$ one could *formally* write $q(f, g) = (f, Ag)$ where $A: g \mapsto \delta(x)g(x)$. Since multiplication by $\delta(x)$ is not an operator, q is an example of a quadratic form not likely to be associated with an operator.

Example 2 Let A be a self-adjoint operator on $\mathscr{H}$. Let us pass to a spectral representation of A, so that A is multiplication by x on $\bigoplus_{n=1}^N L^2(\mathbb{R}, \mu_n)$. Let

$$Q(q) = \left\{ \{\psi_n(x)\}_{n=1}^N \;\middle|\; \sum_{n=1}^N \int_{-\infty}^{\infty} |x|\,|\psi_n(x)|^2 \, d\mu_n < \infty \right\}$$

and for $\psi, \varphi \in Q(q)$ define

$$q(\varphi, \psi) = \sum_{n=1}^N \int_{-\infty}^{\infty} x\overline{\varphi_n(x)}\psi_n(x)\, d\mu_n$$

We call q the **quadratic form** associated with A and write $Q(q) = Q(A)$; $Q(A)$ is called the **form domain of the operator** A. For $\psi, \varphi \in Q(A)$, we will often write $q(\varphi, \psi) = (\varphi, A\psi)$ although A does not make sense on all $\psi \in Q(A)$. $Q(A)$ is in some sense the largest domain on which q can be defined.

To investigate the deep connection between self-adjointness and semibounded quadratic forms we need to extend the notion of "closed" from operators to forms. An operator A is closed if and only if its graph is closed which is the same as saying that $D(A)$ is complete under the norm $\|\psi\|_A = \|A\psi\| + \|\psi\|$ (Problem 15). Analogously, we define:

Definition Let q be a semibounded quadratic form, $q(\psi, \psi) \geq -M\|\psi\|^2$. q is called **closed** if $Q(q)$ is complete under the norm

$$\|\psi\|_{+1} = \sqrt{q(\psi, \psi) + (M+1)\|\psi\|^2}$$

If q is closed and $D \subset Q(q)$ is dense in $Q(q)$ in the $\|\cdot\|_{+1}$ norm, then D is called a **form core** for q.

Notice that $\|\psi\|_{+1}$ comes from the inner product

$$(\psi, \varphi)_{+1} = q(\psi, \varphi) + (M+1)(\psi, \varphi)$$

It is not hard to see (Problem 15) that q is closed if and only if whenever $\varphi_n \in Q(q)$, $\varphi_n \xrightarrow{\mathscr{H}} \varphi$ and $q(\varphi_n - \varphi_m, \varphi_n - \varphi_m) \to 0$, as $n, m \to \infty$, then $\varphi \in Q(q)$ and $q(\varphi_n - \varphi, \varphi_n - \varphi) \to 0$. This criterion and the dominated convergence

theorem show that the form q associated with a semibounded self-adjoint operator (Example 2) is closed. Furthermore, any operator core for A is a form core for q (Problem 16).

Now, let $q(f, g) = \bar{f}(0)g(0)$ as in Example 1 and φ_n be the C_0^∞ function shown in Figure VIII.2. Then $\varphi_n \overset{\mathscr{H}}{\to} 0$, and $q(\varphi_n - \varphi_m, \varphi_n - \varphi_m) \to 0$, but $q(\varphi_n, \varphi_n) \to 1 \neq q(0, 0)$ which proves that q has no closed extensions. Therefore, even though q is positive (and therefore symmetric) there is no semibounded self-adjoint operator A so that $q(f, g) = (f, Ag)$ for all $f, g \in C_0^\infty$.

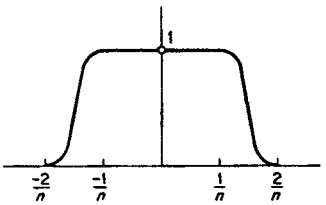

FIGURE VIII.2 The graph of φ_n.

The deep fact about semibounded quadratic forms is that *unlike* the case for operators, they cannot be closed and symmetric, yet not self-adjoint.

Theorem VIII.15 If q is a closed semibounded quadratic form, then q is the quadratic form of a unique self-adjoint operator.

Proof We may assume without loss of generality that q is positive. Then, since q is closed and symmetric, $Q(q)$ is a Hilbert space, which we denote by $\mathscr{H}_{+1}$, under the inner product

$$(\varphi, \psi)_{+1} = q(\varphi, \psi) + (\varphi, \psi)$$

We denote by $\mathscr{H}_{-1}$ the space of bounded conjugate linear functionals on $\mathscr{H}_{+1}$. Let j, given by $\psi \overset{j}{\mapsto} (\cdot, \psi)$, be the linear imbedding of $\mathscr{H}$ into $\mathscr{H}_{-1}$. $j(\psi)$ is bounded because

$$|[j(\psi)](\varphi)| \leq \|\varphi\| \|\psi\| \leq \|\varphi\|_{+1} \|\psi\|$$

Since the identity map i embeds $\mathscr{H}_{+1}$ in $\mathscr{H}$ we have a "scale of spaces"

$$\mathscr{H}_{+1} \overset{i}{\to} \mathscr{H} \overset{j}{\to} \mathscr{H}_{-1}$$

We now exploit the Riesz lemma. Given $\Phi \in \mathscr{H}_{+1}$, let $\hat{B}\Phi$ be the element of $\mathscr{H}_{-1}$ which acts by

$$[\hat{B}\Phi](\varphi) = q(\varphi, \Phi) + (\varphi, \Phi)$$

By the Riesz lemma, $\hat{B}$ is an isometric isomorphism of $\mathscr{H}_{+1}$ onto $\mathscr{H}_{-1}$. Let $D(B) = \{\psi \in \mathscr{H}_{+1} \mid \hat{B}\psi \in \operatorname{Ran} j\}$. Define B on $D(B)$ by $B = j^{-1}\hat{B}$.

$$\mathscr{H} \supset \mathscr{H}_{+1} \xrightarrow{\hat{B}} \mathscr{H}_{-1} \xleftarrow{j} \mathscr{H}$$

First, we prove that the range of j is dense in $\mathscr{H}_{-1}$. If it were not, there would be a $\lambda \in \mathscr{H}_{-1}^{*}$ so that $\lambda \neq 0$, and $\lambda[j(\psi)] = 0$ for each $\psi \in \mathscr{H}$. By the Riesz Lemma, there is a $\varphi_\lambda \neq 0$ in $\mathscr{H}_{+1}$ so that $0 = \lambda[j(\psi)] = [j(\psi)](\varphi_\lambda) = (\varphi_\lambda, \psi)$ for all $\psi \in \mathscr{H}$. Since $\varphi_\lambda \neq 0$, this is impossible. Therefore $\operatorname{Ran} j$ is dense in $\mathscr{H}_{-1}$. Since B is an isometric isomorphism we conclude that $D(B)$ is $\|\cdot\|_{+1}$ dense in $\mathscr{H}_{+1}$. Further, since $\|\cdot\| \leq \|\cdot\|_{+1}$ and $\mathscr{H}_{+1}$ is norm dense in $\mathscr{H}$, $D(B)$ is norm dense in $\mathscr{H}$.

Suppose $\varphi, \psi \in D(B)$. Then

$$\begin{aligned}(\varphi, B\psi) &= q(\varphi, \psi) + (\varphi, \psi) \\ &= \overline{q(\psi, \varphi) + (\psi, \varphi)} \\ &= \overline{(\psi, B\varphi)} \\ &= (B\varphi, \psi)\end{aligned}$$

Thus, B is a densely defined symmetric operator.

We will prove that B is self-adjoint. Let $C = \hat{B}^{-1}j$. C takes $\mathscr{H}$ into $\mathscr{H}$ and is an everywhere defined symmetric operator. By the Hellinger–Toeplitz theorem, C is a bounded self-adjoint operator. Moreover, C is injective. A simple application of the spectral theorem in multiplication operator form shows that C^{-1}: Ran $C \to \mathscr{H}$ is a self-adjoint operator. But $C^{-1} = B$.

We now define $A = B - I$. Then A is also self-adjoint on $D(A) = D(B)$ and for $\varphi, \psi \in D(A)$, $(\varphi, A\psi) = q(\varphi, \psi)$. Since $D(A)$ is $\|\cdot\|_{+1}$-dense in $\mathscr{H}_{+1}$, q is the quadratic form associated to A. Uniqueness is left as a problem. ∎

Thus, there is an interesting distinction between semi-bounded symmetric operators and semi-bounded quadratic forms. For symmetric operators, there is never any problem finding closed extensions. A smallest closed extension always exists (the double adjoint), but it is possible that none of these closed extensions is self-adjoint. On the other hand, semibounded forms need not have any closed extensions, but when such extensions exist and are semi-bounded, they are the quadratic forms associated with self-adjoint operators. We caution the reader about several pitfalls.

(1) If A and B are self-adjoint operators and $D(A) \subset D(B)$ with $B \upharpoonright D(A) = A$, then $A = B$. But it can happen that a and b are closed semi-bounded quadratic forms and $b \upharpoonright Q(a) \times Q(a) = a$ without having $a = b$.

(2) Let A be a symmetric operator that is semibounded. Let q be the quadratic form $q(\varphi, \psi) = (\varphi, A\psi)$ with $Q(a) = D(A)$. Suppose that q has a closure (it always will, see Section X.3) $\hat{q}$, that is, a smallest closed form which extends it. Then the self-adjoint operator $\hat{A}$ which corresponds to $\hat{q}$ (by Theorem VIII.15) may be bigger than the operator closure of A.

(3) While a general quadratic form may have no closed extensions, forms that come directly from semibounded operators always have closures and thus semibounded operators always have self-adjoint extensions: see Section X.3.

The following example illustrates the first two of these phenomena.

Example 3 Let $AC^2[0, 1]$ denote the functions $f \in L^2[0, 1]$ such that f is differentiable, f' is absolutely continuous and $f'' \in L^2[0, 1]$. We define

$$D_0 = \{f \mid f \in AC^2[0, 1], \quad f(0) = f(1) = 0 = f(0) = f(1)\}$$
$$D_{a,b} = \{f \mid f \in AC^2[0, 1], \quad af(0) + f'(0) = 0 = bf(1) + f'(1)\}$$
$$D_{\infty,\infty} = \{f \mid f \in AC^2[0, 1], \quad f(0) = 0 = f(1)\}$$
$$D = \{f \mid f \in AC^2[0, 1]\}$$

and let T_0, $T_{a,b}$, $T_{\infty,\infty}$, and T be the operation $-d^2/dx^2$ with domains D_0, $D_{a,b}$, $D_{\infty,\infty}$, and D respectively. Then

(a) The operators T_0, $T_{a,b}$, $T_{\infty,\infty}$, and T are closed. T_0 is symmetric but not self-adjoint; its adjoint is T.

(b) $T_{a,b}(-\infty < a < \infty, \ -\infty < b < \infty)$ and $T_{\infty,\infty}$ are all distinct self-adjoint extensions of T_0 (there are others!).

(c) If $t_0(\varphi, \psi) = (\varphi, T_0\psi)$ for $\varphi, \psi \in D_0$, the form t_0 has a smallest closed extension $\hat{t}_0$. This extension is the form associated with $T_{\infty,\infty}$ which illustrates the remark (2) above.

(d) The form $t_{a,b}$ associated with $T_{a,b}$ has a form domain $Q(t_{a,b})$ which contains the form domain $Q(t_{\infty,\infty})$ of $t_{\infty,\infty}$, the form associated with $T_{\infty,\infty}$, and $t_{a,b} \restriction Q(t_{\infty,\infty}) = t_{\infty,\infty}$. This illustrates the remark (1) above.

Finally, we extend some of the ideas we have considered to nonsymmetric forms. Our use of the terms "sectorial" and "accretive" is not precisely the standard one (see the Notes).

Definition A quadratic form q is called **strictly m-accretive** if

(i) q is closed in the sense that if $\varphi_n \in Q(q)$, $\varphi_n \to \varphi$, and

$$\lim_{n,m\to\infty} q(\varphi_n - \varphi_m, \varphi_n - \varphi_m) = 0$$

then $\varphi \in Q(q)$ and $q(\varphi_n - \varphi, \varphi_n - \varphi) \to 0$.

(ii) there is a θ, $0 < \theta < \pi/2$, with $|\arg[q(\varphi, \varphi)]| \leq \theta$ for all $\varphi \in Q(q)$.

Now, suppose that q is strictly m-accretive. Define a new quadratic form R_q by

$$R_q(\varphi, \psi) = \frac{1}{4}\Big\{\mathrm{Re}[q(\varphi + \psi, \varphi + \psi)] - \mathrm{Re}[q(\varphi - \psi, \varphi - \psi)] + \frac{1}{i}\mathrm{Re}[q(\varphi + i\psi, \varphi + i\psi)] - \frac{1}{i}\mathrm{Re}[q(\varphi - i\psi, \varphi - i\psi)]\Big\}$$

Notice that $R_q(\varphi, \varphi) = \mathrm{Re}[q(\varphi, \varphi)]$ so R_q is a closed positive form. We can now use R_q to set up a scale of spaces $\mathscr{H}_{+1} \subset \mathscr{H} \subset \mathscr{H}_{-1}$ as was done in the proof of Theorem VIII.15, and obtain a map $\hat{T}: \mathscr{H}_{+1} \to \mathscr{H}_{-1}$ so that $[\hat{T}\Phi](\varphi) = \overline{q(\Phi, \varphi)}$. By using the proof of Theorem VIII.15, and by taking T to be a suitable restriction of $\hat{T}$, one can prove:

Theorem VIII.16 Let q be a strictly m-accretive quadratic form. Then there is a unique operator T on $\mathscr{H}$ such that

(a) T is closed.

(b) $D(T) \subset Q(q)$, and if $\varphi, \psi \in D(T)$, then $q(\varphi, \psi) = (\varphi, T\psi)$. Further, $D(T)$ is a form core for q.

(c) $D(T^*) \subset Q(q)$ and if $\varphi, \psi \in D(T^*)$, then $q(\varphi, \psi) = (T^*\varphi, \psi)$. Further, $D(T^*)$ is a form core for q.

The unique operator T given by the above theorem is called the **operator associated with the form** q. Of course, T is called a **strictly m-accretive operator**. Such operators have spectral properties which result from the properties of the associated forms.

Lemma Let T be a strictly m-accretive operator. Then any λ with $\mathrm{Re}\,\lambda < 0$ is in $\rho(T)$ and $\|(T - \lambda)^{-1}\| \leq (-\mathrm{Re}\,\lambda)^{-1}$.

Proof Let $\lambda = \mu + iv$ with $\mu < 0$. Then

$$\begin{aligned}\|(T-\lambda)\varphi\|^2 &= ((T-\lambda)\varphi, (T-\lambda)\varphi)\\ &= (\|T\varphi\|^2 - 2v\,\mathrm{Im}(\varphi, T\varphi) + v^2\|\varphi\|^2) - 2\mu\,\mathrm{Re}(\varphi, T\varphi) + \mu^2\|\varphi\|^2\\ &\geq \mu^2\|\varphi\|^2\end{aligned}$$

since $\mathrm{Re}(\varphi, T\varphi) \geq 0$ and

$$\begin{aligned}&\|T\varphi\|^2 - 2v\,\mathrm{Im}(\varphi, T\varphi) + v^2\|\varphi\|^2\\ &\quad\geq \|T\varphi\|^2 - 2|v|\,\|T\varphi\|\,\|\varphi\| + v^2\|\varphi\|^2 \geq 0\end{aligned}$$

As a result, $T-\lambda$ is injective and $\mathrm{Ran}(T-\lambda)$ is closed. Similarly,

$$\|(T-\lambda)^*\varphi\| \geq \mu^2\|\varphi\|^2$$

so $(\mathrm{Ran}(T-\lambda))^\perp = \mathrm{Ker}(T-\lambda)^* = 0$. Thus, $T-\lambda$ is invertible and

$$\|(T-\lambda)^{-1}\| \leq (-\mu)^{-1}$$ ∎

Before stating this lemma in slightly extended form as a theorem, we extend the notion of accretive.

Definition A form q is called **strictly *m*-sectorial** if there are complex numbers z and $e^{i\alpha}$, with α real, so that $e^{i\alpha}q + z$ is strictly m-accretive. The operator T associated with q is also called **strictly *m*-sectorial.**

Notice that if q is strictly m-sectorial, then the values of $q(\varphi, \varphi)$ lie in a sector

$$S_q = \{\omega \mid \theta_0 \leq \arg(\omega - z) \leq \theta_1, \qquad \text{with} \quad |\theta_1 - \theta_0| < \pi\}$$

S_q is called a **sector** for q.

Theorem VIII.17 Let q be a strictly m-sectorial form, S_q a sector for q, and T the associated operator. If $\lambda \notin S_q$, then $\lambda \in \rho(T)$ and $\|(T-\lambda)^{-1}\| \leq [\mathrm{dist}(\lambda, S_q)]^{-1}$.

The idea of the proof is to translate and rotate S_q so that $\mathrm{dist}(\lambda, S_q)$ is arbitrarily close to the real part of the translate of λ (see Figure VIII.3).

Example 4 Let H_0 and V be positive self-adjoint operators with $Q(H_0) \cap Q(V)$ dense. Let $Q(h) = Q(H_0) \cap Q(V)$. Given $\beta \in \mathbb{C}\backslash(-\infty, 0)$, define $h(\varphi, \psi) = (\varphi, H_0\psi) + \beta(\varphi, V\psi)$. Then h is closed and is a strictly m-sectorial form so we can use Theorem VIII.17 to gain information about $H = H_0 + \beta V$.

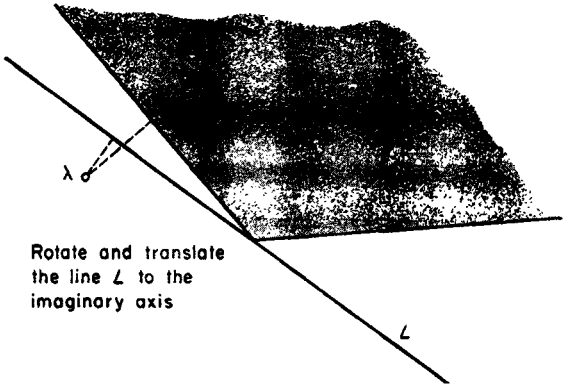

FIGURE VIII.3

In the past, the symbol $A + B$ meant the operator sum defined on $D(A) \cap D(B)$, or perhaps its operator closure. In Example 4, the plus in $H_0 + \beta V$ indicates the operator associated with the sum of *forms* defined on $Q(H_0) \cap Q(V)$. In the future in cases where no confusion can arise we will write $A + B$ without being explicit about the meaning of $+$.

VIII.7 Convergence of unbounded operators †

One of the main difficulties with unbounded operators is that they are only densely defined. This difficulty is especially troublesome when one wants to find a notion of convergence for a sequence $A_n \to A$ of unbounded operators since the domains of the operators A_n may have no vector in common. For example, if $A_n = (1 - 1/n)x$ on $L^2(\mathbb{R})$, it is clear that in some sense $A_n \to A = x$; yet we could have been given domains $D(A_n)$ and $D(A)$ of essential self-adjointness for these operators which have no nonzero vector in common (Problem 19). Of course, in this simple case the closures of A_n and A all have the same domain, but in general this will not be true, and in any case, one is often forced to deal with domains of essential self-adjointness since closures of operators are sometimes difficult to compute. It is very natural to say that self-adjoint operators are "close" if certain bounded functions of them are "close." Most of this section is devoted to this approach. However, we also introduce graph limits, a topic which will be explored further in Section X.8.

† A supplement to this section begins on p. 372.

Definition Let A_n, $n = 1, 2, \ldots$ and A be self-adjoint operators. Then A_n is said to converge to A in the **norm resolvent sense** (or **norm generalized sense**) if $R_\lambda(A_n) \to R_\lambda(A)$ in norm for all λ with $\operatorname{Im} \lambda \neq 0$. A_n is said to converge to A in the **strong resolvent sense** (or **strong generalized sense**) if $R_\lambda(A_n) \to R_\lambda(A)$ strongly for all λ with $\operatorname{Im} \lambda \neq 0$.

We have not introduced the notion of weak resolvent convergence since weak resolvent convergence implies strong resolvent convergence (Problem 20). The following theorem shows that norm resolvent convergence is the right generalization of norm convergence for bounded self-adjoint operators. A similar result holds for strong resolvent convergence (see Problem 28), but the analogue for weak convergence is not true (Problem 30).

Theorem VIII.18 Let $\{A_n\}_{n=1}^{\infty}$ and A be a family of uniformly bounded self-adjoint operators. Then $A_n \to A$ in the norm resolvent sense if and only if $A_n \to A$ in norm.

Proof Let $A_n \to A$ in norm. Then if $\operatorname{Im} \lambda \neq 0$, $(A_n - A)(A - \lambda)^{-1} \to 0$ in norm. Thus, using

$$(A_n - \lambda)^{-1} = (A - \lambda)^{-1}(I + (A_n - A)(A - \lambda)^{-1})^{-1}$$

we see that $(A_n - \lambda)^{-1} \to (A - \lambda)^{-1}$ in norm.

Conversely, suppose $A_n \to A$ in the norm resolvent sense. Then, since

$$A_n - A = (A_n - i)[(A - i)^{-1} - (A_n - i)^{-1}](A - i)$$

and $\sup \|A_n\| < \infty$, we conclude that

$$\begin{aligned} \|A_n - A\| &\leq (\sup \|A_n\| + 1)\|(A - i)^{-1} - (A_n - i)^{-1}\|(\|A\| + 1) \\ &\to 0 \quad \text{as} \quad n \to \infty \end{aligned}$$

∎

The following theorem shows that to prove generalized convergence one need only show convergence of the resolvents at one point off the real axis.

Theorem VIII.19 Let $\{A_n\}_{n=1}^{\infty}$ and A be self-adjoint operators, and let λ_0 be a point in $\mathbb{C}$.

(a) If $\operatorname{Im} \lambda_0 \neq 0$ and $\|R_{\lambda_0}(A_n) - R_{\lambda_0}(A)\| \to 0$, then $A_n \to A$ in the norm resolvent sense.

(b) If $\operatorname{Im} \lambda_0 \neq 0$ and if $R_{\lambda_0}(A_n)\varphi - R_{\lambda_0}(A)\varphi \to 0$, for all $\varphi \in \mathscr{H}$, then $A_n \to A$ in the strong resolvent sense.

Proof (a) Both $R_\lambda(A)$ and $R_\lambda(A_n)$ are analytic in the half-plane containing λ_0 and have power series around λ_0,

$$R_\lambda(A) = \sum_{m=0}^{\infty} (\lambda_0 - \lambda)^m [R_{\lambda_0}(A)]^{m+1}$$

$$R_\lambda(A_n) = \sum_{m=0}^{\infty} (\lambda_0 - \lambda)^m [R_{\lambda_0}(A_n)]^{m+1}$$

which converge in norm in the circle $|\lambda - \lambda_0| < |\operatorname{Im} \lambda_0|^{-1}$. Since $R_{\lambda_0}(A_n) \to R_{\lambda_0}(A)$ in norm, $R_\lambda(A_n) \to R_\lambda(A)$ in norm for λ in this circle. Therefore, by repeating this process, we get convergence for all λ in the half-plane containing λ_0. Furthermore, since

$$\begin{aligned} \|R_{\bar{\lambda}_0}(A_n) - R_{\bar{\lambda}_0}(A)\| &= \|(R_{\lambda_0}(A_n) - R_{\lambda_0}(A))^*\| \\ &= \|R_{\lambda_0}(A_n) - R_{\lambda_0}(A)\| \\ &\to 0 \qquad \text{as} \quad n \to \infty \end{aligned}$$

the same argument shows that the resolvents converge in norm in the half-plane containing $\bar{\lambda}_0$.

(b) The proof is the same as the proof of (a) except for two things. First, one considers the *vector-valued* functions $R_\lambda(A_n)\varphi$ and $R_\lambda(A)\varphi$. Secondly, since the map $T \to T^*$ is not continuous in the strong topology, one needs a separate argument to get from one half-plane to the other. Suppose that λ_0 is in the lower half-plane. Then, as in (a), we get convergence everywhere in the lower half-plane, in particular at $\lambda = -i$. The formula

$$\begin{aligned} &(A_n - i)^{-1} - (A - i)^{-1} \\ &\quad = [(A_n + i)(A_n - i)^{-1}][(A_n + i)^{-1} - (A + i)^{-1}][(A + i)(A - i)^{-1}] \end{aligned}$$

which follows from elementary manipulations, can then be used to prove that $(A_n - i)^{-1}$ converges strongly to $(A - i)^{-1}$. The above argument then shows that $R_\lambda(A_n)$ converges strongly to $R_\lambda(A)$ everywhere in the upper half-plane. ∎

For alternative ways of proving that strong convergence, $R_\lambda(A_n) \xrightarrow{s} R_\lambda(A)$, in one half-plane implies strong convergence in the other half-plane, see Theorem VIII.26 or Problem 20b.

We will investigate several aspects of generalized convergence. First, we ask how resolvent convergence is related to the convergence of other bounded functions of A_n and A. Secondly, we investigate the relationship between the spectra of A_n and the spectrum of A if $A_n \to A$ in a generalized sense. Finally, we give criteria on the operators A_n, A themselves which are sufficient to guarantee that $A_n \to A$ in a generalized sense.

Theorem VIII.20 Let A_n and A be self-adjoint operators.

(a) If $A_n \to A$ in the norm resolvent sense and f is a continuous function on $\mathbb{R}$ vanishing at ∞, then $\|f(A_n) - f(A)\| \to 0$.

(b) If $A_n \to A$ in the strong resolvent sense and f is a bounded continuous function on $\mathbb{R}$, then $f(A_n)\varphi \to f(A)\varphi$ for all $\varphi \in \mathscr{H}$.

Proof By the Stone–Weierstrass theorem, polynomials in $(x+i)^{-1}$ and $(x-i)^{-1}$ are dense in $C_\infty(\mathbb{R})$, the continuous functions vanishing at infinity. Thus, given $\varepsilon > 0$, we can find a polynomial $P(s, t)$ so that

$$\|f(x) - P((x+i)^{-1}, (x-i)^{-1})\|_\infty \leq \varepsilon/3$$

Therefore,

$$\|f(A_n) - P((A_n+i)^{-1}, (A_n-i)^{-1})\| \leq \varepsilon/3$$

and

$$\|f(A) - P((A+i)^{-1}, (A-i)^{-1})\| \leq \varepsilon/3$$

If $A_n \to A$ in the norm resolvent sense, then

$$P((A_n+i)^{-1}, (A_n-i)^{-1}) \to (P((A+i)^{-1}, (A-i)^{-1})$$

in norm as $n \to \infty$, and thus for n large enough, $\|f(A_n) - f(A)\| \leq \varepsilon$. This proves (a).

To prove (b) we first note that the same proof as above shows that if $A_n \to A$ in the strong resolvent sense and $h \in C_\infty(\mathbb{R})$, then $h(A_n)\varphi \to h(A)\varphi$. Let $\psi \in \mathscr{H}$ and $\varepsilon > 0$ be given and define $g_m(x) = \exp(-x^2/m)$. Since $g_m(x) \uparrow 1$ pointwise, $g_m(A)\psi \to \psi$ by Theorem VIII.5, so we can find an m with $\|g_m(A)\psi - \psi\| \leq \varepsilon(6\|f\|_\infty)^{-1}$. Furthermore since $g_m \in C_\infty(\mathbb{R})$, $g_m(A_n)\psi \to g_m(A)\psi$ by the remark above, so we can find an N_0, so that $n \geq N_0$ implies $\|g_m(A_n)\psi - g_m(A)\psi\| \leq \varepsilon(6\|f\|_\infty)^{-1}$. Therefore, if $n \geq N_0$,

$$\|g_m(A_n)\psi - \psi\| \leq \varepsilon(3\|f\|_\infty)^{-1}$$

Since fg_m is continuous and goes to zero at ∞, there is an N_1 so that $n \geq N_1$ implies

$$\|f(A_n)g_m(A_n)\psi - f(A)g_m(A)\psi\| \leq \varepsilon/3$$

Let $N = \max\{N_0, N_1\}$. Then for $n \geq N$,

$$\begin{aligned}\|f(A_n)\psi - f(A)\psi\| &\leq \|f(A_n)g_m(A_n)\psi - f(A)g_m(A)\psi\| \\ &\quad + \|f(A_n)\|\,\|g_m(A_n)\psi - \psi\| \\ &\quad + \|f(A)\|\,\|g_m(A)\psi - \psi\| \\ &\leq \varepsilon\end{aligned}$$

Since ψ and ε were arbitrary, this proves (b). ∎

As an example of an application of part (a) let $\{A_n\}$ and A be positive self-adjoint operators. Then, if $A_n \to A$ in the norm resolvent sense e^{-tA_n} converges in norm to e^{-tA} for each positive t. To see that part (a) does not extend to all of $C(\mathbf{R})$, notice that on $L^2(\mathbf{R})$ the operators $A_n = (1 - 1/n)x$ converge to the operator $A = x$ in the norm resolvent sense but $\|e^{itA_n} - e^{itA}\| = 1$ for all n.

A very important application of part (b) is the following theorem.

Theorem VIII.21 (Trotter) Let $\{A_n\}$ and A be self-adjoint operators. Then $A_n \to A$ in the strong resolvent sense if and only if e^{itA_n} converges strongly to e^{itA} for each t.

Proof Since e^{itx} is a bounded continuous function of x, Theorem VIII.20 implies that if $A_n \to A$ in the strong resolvent sense, then $e^{itA_n} \to e^{itA}$ strongly for each t.

To prove the theorem in the other direction, we first derive a formula for the resolvent of a self-adjoint operator A. Suppose that $\operatorname{Im} \mu < 0$. Then, by the functional calculus

$$\begin{aligned}
(\psi, R_\mu(A)\varphi) &= \int_{-\infty}^{\infty} \left(\frac{1}{\mu - \lambda}\right) d(\psi, P_\lambda \varphi) \\
&= \int_{-\infty}^{\infty} \left(i \int_0^{\infty} e^{-it\mu} e^{it\lambda}\, dt \right) d(\psi, P_\lambda \varphi) \\
&= i \int_0^{\infty} e^{-it\mu} \left(\int_{-\infty}^{\infty} e^{it\lambda}\, d(\psi, P_\lambda \varphi) \right) dt \\
&= i \int_0^{\infty} e^{-it\mu} (\psi, e^{itA}\varphi)\, dt \\
&= \left(\psi, i \int_0^{\infty} e^{-it\mu} e^{itA}\varphi\, dt \right)
\end{aligned}$$

Therefore,

$$R_\mu(A)\varphi = i \int_0^{\infty} e^{-it\mu} e^{itA}\varphi\, dt \tag{VIII.9}$$

where the integral is a Riemann integral. The third step in the computation uses Fubini's theorem. Applying (VIII.9) to the operators A_n and A

$$\|R_\mu(A_n)\varphi - R_\mu(A)\varphi\| \leq \int_0^{\infty} e^{(\operatorname{Im}\mu)t} \|e^{itA_n}\varphi - e^{itA}\varphi\|\, dt$$

so if $e^{itA_n}\varphi \to e^{itA}\varphi$ for each t,

$$\|R_\mu(A_n)\varphi - R_\mu(A)\varphi\| \to 0$$

by the Lebesgue dominated convergence theorem. Using a formula similar to (VIII.9) one concludes in the same way that

$$\| R_\mu(A_n)\varphi - R_\mu(A)\varphi \| \to 0 \qquad \text{for} \quad \operatorname{Im} \mu > 0 \ \blacksquare$$

We remark that it is possible to show (Problem 21) that if $A_n \to A$ in the strong resolvent sense, then $e^{itA_n}\varphi \to e^{itA}\varphi$ for each φ, *uniformly* for t in any finite interval. Next, we prove a related theorem.

Theorem VIII.22 (Trotter–Kato) Let A_n be a sequence of self-adjoint operators. Suppose that there exist points, λ_0 in the upper half-plane and μ_0 in the lower half-plane, so that $R_{\lambda_0}(A_n)\varphi$ and $R_{\mu_0}(A_n)\varphi$ converge for each $\varphi \in \mathscr{H}$. Suppose further that one of the limiting operators, T_{λ_0} or T_{μ_0}, has a dense range. Then there exists a self-adjoint operator A so that $A_n \to A$ in the strong resolvent sense.

Proof Since $\|R_{\lambda_0}(A_n)\| \leq |\operatorname{Im} \lambda_0|^{-1}$, $\|T_{\lambda_0}\| \leq |\operatorname{Im} \lambda_0|^{-1}$, and so

$$T_\lambda = \sum_{n=0}^{\infty} (\lambda_0 - \lambda)^n (T_{\lambda_0})^{n+1}$$

is well defined for $|\lambda - \lambda_0| \leq |\operatorname{Im} \lambda_0|^{-1}$.

Furthermore, since $R_{\lambda_0}(A_n)\varphi \to T_{\lambda_0}\varphi$, $R_\lambda(A_n)\varphi \to T_\lambda\varphi$ in the same circle. Continuing in this way we can define an analytic operator valued function T_λ in the half-plane containing λ_0 which is the strong limit of $R_\lambda(A_n)$. Since the half-plane is simply connected, the determination of T_λ at a point λ is independent of the path taken from λ_0 to λ. The same argument for the half-plane containing μ_0 shows that we can extend the definition of T_λ to that half-plane so that

$$T_\lambda \varphi = \lim_{n \to \infty} R_\lambda(A_n)\varphi \qquad \forall \lambda \text{ with } \operatorname{Im} \lambda \neq 0$$

The T_λ commute, satisfy the first resolvent equation, and $T_\lambda^* = T_{\bar{\lambda}}$ since these statements are true for each $R_\lambda(A_n)$. It follows from the first resolvent formula and the commutativity that the ranges of all the T_λ are equal; we denote this common range by D. By hypothesis, D is dense and this implies that the kernel of T_λ is empty, since $\operatorname{Ker} T_\lambda = (\operatorname{Ran} T_\lambda^*)^\perp = (\operatorname{Ran} T_{\bar{\lambda}})^\perp = D^\perp = \{0\}$. We can therefore define $A = \lambda I - T_\lambda^{-1}$ on D and a short calculation with the resolvent equation shows that this definition is independent of which λ, with $\operatorname{Im} \lambda \neq 0$, is chosen. Since $\operatorname{Ran}(A \pm i) = \operatorname{Ran}(-T_{\mp i}^{-1}) = \mathscr{H}$, A is self-adjoint. It is clear that the resolvent of A is T_λ. $\blacksquare$

Notice that in the Trotter–Kato theorem we need convergence at *two* points, one in the upper half-plane and one in the lower half-plane. For, we

cannot use Theorem VIII.19b until we know that the limiting operator is self-adjoint, and the self-adjointness proof depends on the convergence in both half-planes.

The Trotter–Kato theorem is important since its hypotheses do *not* assume the a priori existence of a limiting operator A. It can be used to assert the existence of a generalized limit of a sequence of self-adjoint operators. This can also be done with the one-parameter groups (see Problem 23). To see why it is necessary to use the resolvents or groups rather than the operators themselves to prove such an existence theorem consider the following example: Let A be a closed symmetric operator which is not self-adjoint but which has a self-adjoint extension $\tilde{A}$. Let P_n be the spectral projection of $\tilde{A}$ corresponding to the interval $[-n, n]$. Then $P_n \tilde{A} P_n$ are bounded self-adjoint operators (and therefore essentially self-adjoint on $D(A)$) such that for all $\varphi \in D(A)$

$$P_n \tilde{A} P_n \varphi \to \tilde{A}\varphi = A\varphi$$

Thus the $P_n \tilde{A} P_n$ are essentially self-adjoint on $D(A)$ and the strong limit exists but the limit is not essentially self-adjoint.

One of the most useful aspects of generalized convergence is that the spectra and projections of the A_n are related to the spectrum and projections of A. For applications of the following two theorems see Sections X.2 and XI.5.

Theorem VIII.23 Let $\{A_n\}_{n=1}^{\infty}$ and A be self-adjoint operators and suppose that $A_n \to A$ in the norm resolvent sense. Then

(a) If $\mu \notin \sigma(A)$, then $\mu \notin \sigma(A_n)$ for n sufficiently large and

$$\|R_\mu(A_n) - R_\mu(A)\| \to 0$$

(b) Let $a, b \in \mathbb{R}$, $a < b$, and suppose that $a \in \rho(A)$, $b \in \rho(A)$. Then

$$\|P_{(a,b)}(A_n) - P_{(a,b)}(A)\| \to 0$$

Proof (a) We need only consider the case where μ is real. Since $\mu \in \rho(A)$, there is a $\delta > 0$ so that $(\mu - \delta, \mu + \delta) \cap \sigma(A) = \varnothing$. Thus, by the functional calculus, $\|R_{\mu + i\delta/3}(A)\| < 1/\delta$. Now, we can find N so that

$$\|R_{\mu + i\delta/3}(A_n)\| \leq 2/\delta$$

for $n \geq N$, which implies that the power series for $R_\lambda(A_n)$ about $\mu + i\delta/3$ has radius of convergence at least $\delta/2$. We already know that where the series converges it is an inverse for A_n. So, $\mu \in \rho(A_n)$ for $n \geq N$ and

$$\|R_\mu(A_n) - R_\mu(A)\| \to 0$$

To prove (b), we note that since $a, b \in \rho(A)$, there exists $\varepsilon < \frac{1}{2}(b-a)$ and an N, so that

$$\sup_{n \geq N} \{\|(A_n - a)^{-1}\|, \|(A_n - b)^{-1}\|\} \leq 1/\varepsilon$$

Therefore, by the functional calculus, $\sigma(A_n) \cap (a, b) \subset (a + \varepsilon, b - \varepsilon)$ for $n \geq N$. Let f be a continuous function which equals one on $(a + \varepsilon, b - \varepsilon)$ and is equal to zero outside (a, b). Then

$$P_{(a,b)}(A_n) = f(A_n) \qquad P_{(a,b)}(A) = f(A)$$

and so by Theorem VIII.20,

$$\|P_{(a,b)}(A_n) - P_{(a,b)}(A)\| \to 0 \quad \blacksquare$$

Theorem VIII.24 Let $\{A_n\}_{n=1}^{\infty}$ and A be self-adjoint operators and suppose that $A_n \to A$ in the strong resolvent sense. Then

(a) If $a, b \in \mathbb{R}$, $a < b$, and $(a, b) \cap \sigma(A_n) = \varnothing$ for all n, then $(a, b) \cap \sigma(A) = \varnothing$. That is, if $\lambda \in \sigma(A)$, then there exists $\lambda_n \in \sigma(A_n)$ so that $\lambda_n \to \lambda$.

(b) If $a, b \in \mathbb{R}$, $a < b$, and $a, b \notin \sigma_{\text{pp}}(A)$, then $P_{(a,b)}(A_n)\varphi \to P_{(a,b)}(A)\varphi$ for all $\varphi \in \mathscr{H}$.

Proof By the functional calculus, the statement that $(a, b) \cap \sigma(A) = \varnothing$ is equivalent to the statement that

$$\|(A - \lambda_0)^{-1}\| \leq \frac{\sqrt{2}}{b-a}$$

where

$$\lambda_0 = \frac{a+b}{2} + i\left(\frac{b-a}{2}\right)$$

But $(A_n - \lambda_0)^{-1}$ converges strongly to $(A - \lambda_0)^{-1}$ so we have

$$\|(A-\lambda_0)^{-1}\| \leq \varliminf_n \|(A_n-\lambda_0)^{-1}\| \leq \frac{\sqrt{2}}{b-a}$$

This proves (a).

To prove (b), we find uniformly bounded sequences of continuous functions f_n and g_n so that $0 \leq f_n \leq \chi_{(a,b)}$, $f_n(x) \nearrow \chi_{(a,b)}(x)$ pointwise and $\chi_{[a,b]} \leq g_n$, $g_n(x) \searrow \chi_{[a,b]}(x)$ pointwise. Then $f_n(A) \to P_{(a,b)}(A)$ and $g_n(A) \to P_{[a,b]}(A)$ strongly.

Since $a, b \notin \sigma_{pp}(A)$, $P_{[a,b]}(A) = P_{(a,b)}(A)$ which means that given ψ and $\varepsilon > 0$, we can find continuous functions f, g, with $f \leq \chi_{(a,b)} \leq \chi_{[a,b]} \leq g$, so that $\|f(A)\psi - g(A)\psi\| \leq \varepsilon/5$. By Theorem VIII.20b we can find N so that $n \geq N$ implies

$$\|f(A_n)\psi - f(A)\psi\| \leq \varepsilon/5 \qquad \|g(A_n)\psi - g(A)\psi\| \leq \varepsilon/5$$

so by an $\varepsilon/3$ argument

$$\|f(A_n)\psi - g(A_n)\psi\| \leq 3\varepsilon/5$$

Since the functional calculus implies

$$\|f(A)\psi - P_{(a,b)}(A)\psi\| \leq \|f(A)\psi - g(A)\psi\|$$

another $\varepsilon/3$ argument implies

$$\|P_{(a,b)}(A_n)\psi - P_{(a,b)}(A)\psi\| \leq \varepsilon \ \blacksquare$$

Part (a) of Theorem VIII.24 says that the spectrum of the limiting operator cannot suddenly expand. It can, however, contract rather spectacularly as the following example shows: Let $A_n = x/n$ on $L^2(\mathbb{R})$; then A_n converges to the zero operator in the strong resolvent sense. For each n, $\sigma(A_n) = \mathbb{R}$, but the spectrum of the limiting operator contains only the origin. An easy application of part (a) is the statement that if the A_n are positive and $A_n \to A$ in the strong resolvent sense, then A is positive.

If A_n converges to A in *norm* resolvent sense, Theorem VIII.23 tells us that the spectrum of the limiting operator cannot suddenly contract in the sense that if $\lambda \in \sigma(A_n)$ for all sufficiently large n, then $\lambda \in \sigma(A)$. Notice that in the example $A_n = x/n$ above, A_n does not converge to A in the norm resolvent sense.

The principle of noncontraction of the spectrum under norm resolvent convergence remains true even when A_n and A are not self-adjoint. But the principle of nonexpansion of the spectrum in the strong resolvent limit is not always valid for general not-necessarily-self-adjoint operators. In fact, there exists a *norm* convergent sequence of uniformly bounded operators $A_n \to A$ with $\sigma(A_n)$ the unit circle in $\mathbb{C}$ for each n and $\sigma(A)$ the entire unit disc. Thus the reader should be careful to apply Theorem VIII.24 only in the self-adjoint case.

In applications, one is usually given the operators $\{A_n\}$ and A on domains of self-adjointness or essential self-adjointness and it may be very difficult to compute the resolvents. Thus, in order to use Theorems VIII.23 and VIII.24 one must have criteria on the operators A_n, A themselves which guarantee norm or strong resolvent convergence.

Theorem VIII.25 (a) Let $\{A_n\}_{n=1}^{\infty}$ and A be self-adjoint operators and suppose that D is a common core for all A_n, A. If $A_n\varphi \to A\varphi$ for each $\varphi \in D$, then $A_n \to A$ in the strong resolvent sense.

(b) Let $\{A_n\}_{n=1}^{\infty}$ and A be self-adjoint operators with a common domain, D. Norm D with $\|\varphi\|_A = \|A\varphi\| + \|\varphi\|$. If

$$\sup_{\|\varphi\|_A = 1} \|(A_n - A)\varphi\| \to 0$$

then $A_n \to A$ in the norm resolvent sense.

(c) Let $\{A\}_{n=1}^{\infty}$ and A be positive self-adjoint operators with a common form domain $\mathscr{H}_{+1}$ which we norm with

$$\|\psi\|_{+1} = \sqrt{(\psi, A\psi) + (\psi, \psi)}$$

If $A_n \to A$ in norm in the sense of maps from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$, that is, if

$$\sup_{0\neq\psi,\,\varphi\in D} \frac{|(\varphi, (A - A_n)\psi)|}{\|\varphi\|_{+1}\|\psi\|_{+1}} = \sup_{0\neq\psi\in D} \frac{|(\psi, (A - A_n)\psi)|}{(\psi, (A+1)\psi)} \longrightarrow 0$$

then $A_n \to A$ in the norm resolvent sense.

Proof (a) Let $\varphi \in D$, $\psi = (A + i)\varphi$, then

$$[(A_n + i)^{-1} - (A + i)^{-1}]\psi = (A_n + i)^{-1}(A - A_n)\varphi$$

converges to zero as $n \to \infty$, since $(A - A_n)\varphi \to 0$ and the $(A_n + i)^{-1}$ are uniformly bounded. Since D is a core for A, the set of such ψ is dense so

$$(A_n + i)^{-1}\varphi \to (A + i)^{-1}\varphi \qquad \text{for all} \quad \varphi \in \mathscr{H}$$

A similar proof works for $(A_n - i)^{-1}$.

We sketch the proofs of (b) and (c). For (b), first one proves that the hypothesis is equivalent to $(A_n - A)(A + i)^{-1} \to 0$ in the ordinary $\mathscr{H}$-operator norm. Thus $(I + (A_n - A)(A + i)^{-1})^{-1}$ exists and converges to I in norm as $n \to \infty$. As a result

$$(A_n + i)^{-1} = (A + i)^{-1}(I + (A_n - A)(A + i)^{-1})^{-1} \to (A + i)^{-1}$$

in norm. Similarily $(A_n - i)^{-1} \to (A - i)^{-1}$.

To prove (c), one first proves that the hypothesis is equivalent to

$$(A + I)^{-1/2}(A_n - A)(A + I)^{-1/2} \to 0$$

in the ordinary operator norm. Using

$$(A_n + I)^{-1} = (A + I)^{-1/2}(I + (A + I)^{-1/2}(A_n - A)(A + I)^{-1/2})^{-1}(A + I)^{-1/2}$$

one then follows the proof of (b). ∎

Finally, we introduce graph limits and compare them with generalized limits. Graph limits will be discussed again in Section X.8.

Definition Let A_n be a sequence of operators on a Hilbert space $\mathscr{H}$. We say that $\langle \psi, \varphi \rangle \in \mathscr{H} \times \mathscr{H}$ is in the **strong graph limit** of A_n if we can find $\psi_n \in D(A_n)$ so that $\psi_n \to \psi$, $A_n \psi_n \to \varphi$. We denote the set of pairs in the strong graph limit by Γ_∞^s. If Γ_∞^s is the graph of an operator A we say that A is the **strong graph limit** of A_n and write $A = \text{st. gr.-lim } A_n$.

First, we consider the case where all the A_n are self-adjoint *and A is also self-adjoint.*

Theorem VIII.26 Suppose that $\{A_n\}$ and A are self-adjoint operators. Then $A_n \to A$ in the strong resolvent sense if and only if $A = \text{st. gr.-lim } A_n$.

Proof Suppose first that $(A_n + i)^{-1} \to (A + i)^{-1}$ strongly. Suppose $\varphi \in D(A)$. Then $\varphi_n \equiv (A_n + i)^{-1}(A + i)\varphi \to \varphi$ and $A_n\varphi_n = (A + i)\varphi - i\varphi_n \to A\varphi$, so $\langle \varphi, A\varphi \rangle \in \Gamma_\infty^s$. Thus $\Gamma(A) \subset \Gamma_\infty^s$. On the other hand, suppose $\varphi_n \in D(A_n)$, $\varphi_n \to \varphi$ and $A_n\varphi_n \to \psi$. If we let $\eta_n = (A + i)^{-1}(A_n + i)\varphi_n \in D(A)$, then

$$\begin{aligned}
\eta_n - \varphi_n &= [(A + i)^{-1} - (A_n + i)^{-1}][(A_n + i)\varphi_n] \\
&= [(A + i)^{-1} - (A_n + i)^{-1}][(A_n + i)\varphi_n - \psi - i\varphi] \\
&\quad + [(A + i)^{-1} - (A_n + i)^{-1}][\psi + i\varphi] \\
&\to 0 \qquad \text{as} \quad n \to \infty
\end{aligned}$$

Thus, $\eta_n \to \varphi$ and $A\eta_n = (A_n + i)\varphi_n - i\eta_n \to \psi$, so since A is closed $\langle \varphi, \psi \rangle \in \Gamma(A)$. Thus, $\Gamma(A) = \Gamma_\infty^s$.

Conversely, suppose that $A = \text{st. gr.-lim } A_n$. Let $\varphi \in D(A)$. Then there exist $\varphi_n \in D(A_n)$ so that $\varphi_n \to \varphi$ and $A_n\varphi_n \to A\varphi$. Thus,

$$\begin{aligned}
&[(A_n + i)^{-1} - (A + i)^{-1}](A + i)\varphi \\
&\quad = (A_n + i)^{-1}[(A + i)\varphi - (A_n + i)\varphi_n] - (\varphi - \varphi_n) \\
&\quad \to 0 \qquad \text{as} \quad n \to \infty
\end{aligned}$$

since $\|(A_n + i)^{-1}\| \leq 1$, $(A_n + i)\varphi_n \to (A + i)\varphi$, and $\varphi_n \to \varphi$. Since $\text{Ran}(A + i) = \mathscr{H}$, the strong convergence of $(A_n + i)^{-1}$ to $(A + i)^{-1}$ follows. ∎

Thus, we see that *if the limit is self-adjoint*, then strong graph and strong resolvent convergence are the same. It is in the case when we do not know a priori that the limit is self-adjoint that strong graph limits are particularly

interesting. For example, in Section X.8 we will see that the existence of graph limits can sometimes be combined with other information to prove that the limit is self-adjoint.

Theorem VIII.27 Let $\{A_n\}$ be a sequence of symmetric operators.

(a) Let $D_\infty^s = \{\psi \mid \langle \psi, \varphi \rangle \in \Gamma_\infty^s \text{ for some } \varphi\}$. If D_∞^s is dense, then Γ_∞^s is the graph of an operator.

(b) Suppose that D_∞^s is dense and let $A = \text{st. gr.-lim } A_n$.

Then A is symmetric and closed.

Proof We will prove (a); the proof of (b) is left as an exercise (Problem 24). Suppose $\varphi_n, \varphi_n' \in D(A_n)$ and $\varphi_n \to \varphi$, $\varphi_n' \to \varphi$, $A_n\varphi_n \to \psi$, and $A_n\varphi_n' \to \psi'$. Let $\eta \in D_\infty^s$. Then there is an $\eta_n \in D(A_n)$, so that $\eta_n \to \eta$ and $A_n\eta_n \to \rho$. Thus,

$$\begin{aligned}(\psi - \psi', \eta) &= \lim_{n\to\infty} (A_n(\varphi_n - \varphi_n'), \eta_n) \\ &= \lim_{n\to\infty} (\varphi_n - \varphi_n', A_n\eta_n) \\ &= 0\end{aligned}$$

so $\psi = \psi'$, since D_∞^s is dense. ∎

One can also define weak graph limits. We give the definition and state one theorem.

Definition Let A_n be a sequence of operators on $\mathscr{H}$. We say that $\langle \psi, \varphi \rangle \in \mathscr{H} \times \mathscr{H}$ is in the **weak graph limit** Γ_∞^w if we can find $\psi_n \in D(A_n)$ so that $\psi_n \xrightarrow{\|\cdot\|} \psi$ and $A_n\psi_n \to \varphi$ weakly. If Γ_∞^w is the graph of an operator, A, we say that A is the **weak graph limit** of A_n; $A = \text{w. gr.-lim } A_n$.

Theorem VIII.28 Let A_n be a sequence of symmetric operators. If

$$D_\infty^w = \{\psi \mid \{\psi, \varphi\} \in \Gamma_\infty^w \quad \text{for some } \varphi\}$$

is dense, then Γ_∞^w is the graph of a symmetric operator.

Finally we note that if A_n is a uniformly bounded sequence of operators then $A = \text{w. gr.-lim } A_n$ if and only if $A_n \to A$ in the weak operator topology (Problem 26). This fact combined with Problems 20 and 28 shows that the notions of weak graph limit and weak resolvent convergence are distinct. It is not true that weak graph limits are necessarily closed if each A_n is symmetric.

VIII.8 The Trotter product formula†

In this section we prove a useful approximation theorem for $\exp t(A+B)$ in terms of $\exp tA$ and $\exp tB$. It is illuminating to first consider finite-dimensional matrices for which one has the classical theorem of Lie:

Theorem VIII.29 (Lie product formula) Let A and B be finite-dimensional matrices. Then

$$\exp(A+B) = \lim_{n\to\infty} [\exp(A/n)\exp(B/n)]^n$$

Proof Let $S_n = \exp[(A+B)/n)]$, $T_n = \exp(A/n)\exp(B/n)$. Then

$$S_n^n - T_n^n = \sum_{m=0}^{n-1} S_n^m (S_n - T_n) T_n^{n-1-m}$$

so

$$\begin{aligned}\|S_n^n - T_n^n\| &\le n(\max\{\|S_n\|, \|T_n\|\})^{n-1}\|S_n - T_n\| \\ &\le n\|S_n - T_n\|\exp(\|A\| + \|B\|)\end{aligned}$$

Since

$$\|S_n - T_n\| = \left\| \sum_{m=0}^{\infty} \frac{1}{m!}\left(\frac{A+B}{n}\right)^m - \left(\sum_{m=0}^{\infty}\frac{1}{m!}\left(\frac{A}{n}\right)^m\right)\left(\sum_{m=0}^{\infty}\frac{1}{m!}\left(\frac{B}{n}\right)^m\right)\right\|$$

$$\le C/n^2 \qquad (C \text{ depends on } \|A\| \text{ and } \|B\|)$$

we conclude that $\|S_n^n - T_n^n\| \to 0$. ∎

This theorem *and its proof* can be extended to the case where A and B are unbounded self-adjoint operators and $A+B$ is *self-adjoint* on $D(A) \cap D(B)$.

Theorem VIII.30 Let A and B be self-adjoint operators on $\mathscr{H}$ and suppose that $A+B$ is self-adjoint on $D = D(A) \cap D(B)$. Then

$$\text{s-lim}_{n\to\infty} [e^{itA/n}e^{itB/n}]^n = e^{it(A+B)}$$

Proof Let $\psi \in D$. Then

$$s^{-1}(e^{isA}e^{isB} - I)\psi = s^{-1}(e^{isA} - I)\psi + s^{-1}e^{isA}(e^{isB} - I)\psi \to iA\psi + iB\psi$$

and

$$s^{-1}(e^{is(A+B)} - I)\psi \to i(A+B)\psi$$

† A supplement to this section begins on p. 377.

as $s \to 0$. Letting $K(s) = s^{-1}(e^{isA}e^{isB} - e^{is(A+B)})$ we see that $K(s)\psi \to 0$ as $s \to 0$, for each $\psi \in D$. Since $A + B$ is self-adjoint on D, D is a Banach space under the norm

$$\|\psi\|_{A+B} = \|(A + B)\psi\| + \|\psi\|$$

Each of the maps $K(s)$: $D \to \mathscr{H}$ is bounded and $K(s)\psi \xrightarrow{\mathscr{H}} 0$ as $s \to 0$ or ∞ for each $\psi \in D$. Thus, we conclude from the uniform boundedness theorem that the $K(s)$ are uniformly bounded, that is, there is a constant C so that

$$\|K(s)\psi\| \leq C\|\psi\|_{A+B} \qquad \text{for all} \quad s \in \mathbb{R} \text{ and } \psi \in D$$

Therefore, an $\varepsilon/3$ argument shows that on $\|\cdot\|_{A+B}$ compact subsets of D, $K(s)\psi \to 0$ uniformly.

Since $A + B$ is self-adjoint on D, $e^{is(A+B)}\psi \in D$ if $\psi \in D$. Moreover, $s \to e^{is(A+B)}\psi$ is a continuous map of $\mathbb{R}$ into D when D is given the $\|\cdot\|_{A+B}$ norm topology. Thus $\{e^{is(A+B)}\psi \mid s \in [-1, 1]\}$ is a $\|\cdot\|_{A+B}$ compact set in D for each fixed ψ.

We are now ready to mimic the proof of the Lie product formula. We know that

$$t^{-1}[e^{itA}e^{itB} - e^{it(A+B)}]e^{is(A+B)}\psi \to 0$$

uniformly for $s \in [-1, 1]$. Therefore, we write

$$[(e^{itA/n}e^{itB/n})^n - (e^{it(A+B)/n})^n]\psi$$

$$= \sum_{k=0}^{n-1} (e^{itA/n}e^{itB/n})^k [e^{itA/n}e^{itB/n} - e^{it(A+B)/n}][e^{it(A+B)/n}]^{n-1-k}\psi$$

The norm of the right hand side is less than or equal to

$$|t| \max_{|s|<t} \left\| \left(\frac{t}{n}\right)^{-1} (e^{it(A+B)/n} - e^{itA/n}e^{itB/n})e^{is(A+B)}\psi \right\|$$

and so we conclude that

$$(e^{itA/n}e^{itB/n})^n\psi \xrightarrow{\mathscr{H}} e^{it(A+B)}\psi, \qquad \text{as } n \to \infty \quad \text{if } \psi \in D$$

Since D is dense and the operators are bounded by one, this statement holds on all of $\mathscr{H}$. ∎

The above proof shows that on a fixed vector the convergence is uniform for t in a compact subset of $\mathbb{R}$.

The same argument can be used to show that

$$\text{s-lim}_{n\to\infty} (e^{-tA/n}e^{-tB/n})^n = e^{-t(A+B)}$$

if A and B satisfy the same hypotheses and in addition are semibounded. The following result is considerably stronger than Theorem VIII.30 since it only requires *essential* self-adjointness of $A + B$ on $D(A) \cap D(B)$. The proof is quite different from the proof of Theorem VIII.30 (see the notes for references).

Theorem VIII.31 (the Trotter product formula) If A and B are self-adjoint operators and $A + B$ is essentially self-adjoint on $D(A) \cap D(B)$, then

$$\text{s-lim}_{n\to\infty} (e^{itA/n}e^{itB/n})^n = e^{i(A+B)t}$$

Moreover, if A and B are bounded from below, then

$$\text{s-lim}_{n\to\infty} (e^{-tA/n}e^{-tB/n})^n = e^{-t(A+B)}$$

For applications of the Trotter product formula the reader should see Section X.10 (Feynman path integrals), Section X.7 (hypercontractive semigroups), or Chapter XIX (the section on constructive quantum field theory).

VIII.9 The polar decomposition for closed operators

In Section VI.4, we saw that an arbitrary bounded operator T can be written $T = U|T|$ where $|T|$ is positive and self-adjoint and U is a partial isometry. Moreover, the conditions that $\text{Ker}|T| = \text{Ker}\, T$ and that the initial space of U equals $(\text{Ker}\, T)^\perp$ uniquely determine $|T|$ and U. In this section we want to extend this result to *closed* unbounded operators. As in the bounded case, U is easy to construct once $|T|$ has been constructed and, as in the bounded case, we will let $|T| = \sqrt{T^*T}$. In the bounded case, the hard part was the construction of the square root. Now that we have the spectral theorem, it is easy to construct $\sqrt{T^*T}$ if we can prove that T^*T is a positive self-adjoint operator. It is this fact that is hard in the unbounded case. A priori, it is not clear that $\{\psi \mid \psi \in D(T) \text{ and } T\psi \in D(T^*)\}$ is different from $\{0\}$. In fact, this set is dense (Problem 45), but our approach using the theory of semi-bounded quadratic forms does not require us to prove this.

Theorem VIII.32 (the polar decomposition) Let T be an arbitrary closed operator on a Hilbert space $\mathscr{H}$. Then, there is a positive self-adjoint operator $|T|$, with $D(|T|) = D(T)$ and a partial isometry U with initial space,

$(\mathrm{Ker}\ T)^{\perp}$, and final space, $\overline{\mathrm{Ran}\ T}$, so that $T = U|T|$. $|T|$ and U are uniquely determined by these properties together with the additional condition $\mathrm{Ker}(|T|) = \mathrm{Ker}(T)$.

Proof Define the quadratic form s on $D(T)$ by $s(\psi, \phi) = (T\psi, T\phi)$. s is clearly positive. Now suppose $\|\psi_n - \psi_m\|_{+1} \to 0$. Then $\|\psi_n - \psi_m\| \to 0$ and $\|T(\psi_n - \psi_m)\| \to 0$. Since T is closed there is a $\psi \in D(T)$ with $\|\psi_n - \psi\| + \|T(\psi_n - \psi)\| \to 0$, i.e. $\|\psi_n - \psi\|_{+1} \to 0$. Thus s is a closed form. Therefore, by Theorem VIII.15, there is a unique, positive self-adjoint operator S with $Q(S) = D(T)$ and $s(\psi, \phi) = (\psi, S\phi)$ in the sense of forms. Let $|T| = S^{1/2}$. Then $D(|T|) = Q(S) = D(T)$ and by construction $\||T|\psi\|^2 = s(\psi, \psi) = \|T\psi\|^2$ so $\ker|T| = \ker T$. Define U: $\mathrm{Ran}\,|T| \to \mathrm{Ran}\,T$ by $U|T|\psi = T\psi$. Since $\||T|\psi\| = \|T\psi\|$, U is well defined and norm preserving. Thus U extends to a partial isometry from $\overline{\mathrm{Ran}\,|T|}$ to $\overline{\mathrm{Ran}\,T}$. Finally, since $|T|$ is self-adjoint, $\overline{\mathrm{Ran}\,|T|} = (\mathrm{Ker}\,|T|)^{\perp} = (\mathrm{Ker}\,T)^{\perp}$. Uniqueness is left to the reader (Problem 44). ∎

VIII.10 Tensor products

In this section we describe some aspects of the theory of tensor products of operators on Hilbert spaces. Let A and B be densely defined operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$ respectively. We will denote by $D(A) \otimes D(B)$ the set of finite linear combinations of vectors of the form $\phi \otimes \psi$ where $\phi \in D(A)$ and $\psi \in D(B)$. $D(A) \otimes D(B)$ is dense in $\mathscr{H}_1 \otimes \mathscr{H}_2$. We define $A \otimes B$ on $D(A) \otimes D(B)$ by

$$(A \otimes B)(\phi \otimes \psi) = A\phi \otimes B\psi$$

and extend by linearity.

Proposition The operator $A \otimes B$ is well defined. Further, if A and B are closable, so is $A \otimes B$.

Proof Suppose that $\sum c_i \phi_i \otimes \psi_i$ and $\sum d_j \phi'_j \otimes \psi'_j$ are two representations of the same vector $f \in D(A) \otimes D(B)$. Using Gram–Schmidt orthogonalization we can obtain bases $\{\eta_k\}$ and $\{\theta_\ell\}$ for the spaces spanned by $\{\phi_i\} \cup \{\phi'_i\}$ and $\{\psi_j\} \cup \{\psi'_j\}$ respectively so that $\eta_k \in D(A)$ and $\theta_\ell \in D(B)$. $\phi_i \otimes \psi_i$ and $\phi'_j \otimes \psi'_j$ can be expressed

$$\phi_i \otimes \psi_i = \sum \alpha^i_{k\ell} \eta_k \otimes \theta_\ell$$
$$\phi'_j \otimes \psi'_j = \sum \beta^j_{k\ell} \eta_k \otimes \theta_\ell$$

Since the two expressions for f give the same vector, $\sum_i c_i \alpha_{k\ell}^i = \sum_j d_j \beta_{k\ell}^j$ for each pair $\langle k, \ell \rangle$.
Thus,

$$\begin{aligned}(A \otimes B) \sum c_i(\phi_i \otimes \psi_i) &= \sum_{k\ell} \Big(\sum_i c_i \alpha_{k\ell}^i\Big)(A\eta_k \otimes B\theta_\ell) \\ &= \sum_{k\ell} \Big(\sum_j d_j \beta_{k\ell}^j\Big)(A\eta_k \otimes B\theta_\ell) \\ &= (A \otimes B) \sum d_j(\phi_j' \otimes \psi_j')\end{aligned}$$

so $A \otimes B$ is well defined.

If g is any vector in $D(A^*) \otimes D(B^*)$, then $(A \otimes Bf, g) = (f, A^* \otimes B^* g)$ so

$$D(A^*) \otimes D(B^*) \subset D((A \otimes B)^*)$$

If A and B are closable, $D(A^*)$ and $D(B^*)$ are dense. Therefore, in that case $(A \otimes B)^*$ is densely defined which proves that $A \otimes B$ is closable. ∎

Similarly, if A and B are closable then $A \otimes I + I \otimes B$, defined on $D(A) \otimes D(B)$, is closable.

Definition Let A and B be closable operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. The **tensor product** of A and B is the closure of the operator $A \otimes B$ defined on $D(A) \otimes D(B)$. We will denote the closure by $A \otimes B$ also. Usually $A + B$ will denote the closure of $A \otimes I + I \otimes B$ on $D(A) \otimes D(B)$.

Proposition Let A and B be bounded operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. Then $\|A \otimes B\| = \|A\| \, \|B\|$.

Proof Let $\{\phi_k\}$ and $\{\psi_\ell\}$ be orthonormal bases for $\mathscr{H}_1$ and $\mathscr{H}_2$ and suppose $\sum c_{k\ell} \phi_k \otimes \psi_\ell$ is a finite sum. Then

$$\begin{aligned}\|(A \otimes I) \sum c_{k\ell}(\phi_k \otimes \psi_\ell)\|^2 &= \sum_\ell \|\sum_k c_{k\ell} A\phi_k\|^2 \\ &\le \sum_\ell \|A\|^2 \sum_k |c_{k\ell}|^2 \\ &= \|A\|^2 \|\sum c_{k\ell} \phi_k \otimes \psi_\ell\|^2\end{aligned}$$

Since the set of such finite sums is dense in $\mathscr{H}_1 \otimes \mathscr{H}_2$ (Section II.4, Proposition 2), we conclude that $\|A \otimes I\| \le \|A\|$. Thus

$$\|A \otimes B\| \le \|A \otimes I\| \, \|I \otimes B\| \le \|A\| \, \|B\|$$

Conversely, given $\varepsilon > 0$, there exist unit vectors $\phi \in \mathscr{H}_1$, $\psi \in \mathscr{H}_2$ so that $\|A\phi\| \geq \|A\| - \varepsilon$ and $\|B\psi\| \geq \|B\| - \varepsilon$. Then,

$$\begin{aligned}\|(A \otimes B)(\phi \otimes \psi)\| &= \|A\phi\| \, \|B\psi\| \\ &\geq \|A\| \, \|B\| - \varepsilon\|A\| - \varepsilon\|B\| + \varepsilon^2\end{aligned}$$

Since $\varepsilon > 0$ is arbitrary $\|A \otimes B\| \geq \|A\| \, \|B\|$ which concludes the proof. ∎

We remark that both of the above propositions have natural generalizations to arbitrary finite tensor products of operators. This can be proven directly or by using the associativity of the tensor product of Hilbert spaces.

We turn now to questions of self-adjointness and spectrum. Let $\{A_k\}_{k=1}^N$ be a family of operators, A_k self-adjoint on $\mathscr{H}_k$. We will denote the closure of $I_1 \otimes \cdots \otimes A_k \otimes \cdots I$ on $D = \otimes D(A_k)$ by A_k also. Let $P(x_1, \ldots x_N)$ be a polynomial with real coefficients of degree n_k in x_k. Then, the operator $P(A_1, \ldots, A_N)$ makes sense on $\otimes_k D(A^{n_k})$ since $D(A^{n_k}) \subset D(A^\ell)$ for all $\ell \leq n_k$. In fact, P is essentially self-adjoint on that domain.

Theorem VIII.33 Let A_k be a self-adjoint operator on $\mathscr{H}_k$. Let $P(x_1, \ldots, x_N)$ be a polynomial with real coefficients of degree n_k in the kth variable and suppose that D_k^e is a domain of essential self-adjointness for $A_k^{n_k}$. Then,

(a) $P(A_1, \ldots, A_N)$ is essentially self-adjoint on

$$D^e = \bigotimes_{k=1}^N D_k^e$$

(b) The spectrum of $\overline{P(A_1, \ldots, A_N)}$ is the closure of the range of P on the product of the spectra of the A_k. That is

$$\sigma(\overline{P(A_1, \ldots, A_n)}) = \overline{P(\sigma(A_1), \ldots, \sigma(A_N))}$$

Proof We will first prove that $P(A_1, \ldots, A_N)$ is essentially self-adjoint on $D = \otimes_{k=1}^N D(A_k^{n_k})$. By the spectral theorem, there is a measure space $\langle M_k, \mu_k \rangle$ so that A_k is unitarily equivalent to multiplication by a real-valued measurable function f_k on $L^2(M_k, d\mu_k)$. By Proposition 3 in Section VIII.3 we may assume that μ_k is finite and that $f_k \in \bigcap_{1 \leq p < \infty} L^p(M_k, d\mu_k)$. Furthermore, by Theorem II.10(a), $\otimes_{k=1}^N L^2(M_k, d\mu_k)$ is naturally isomorphic to $L^2(\bigtimes_{k=1}^N M_k, \otimes_{k=1} d\mu_k)$. Under this isomorphism $P(A_1, \ldots, A_N)$ corresponds to multiplication by $P(f_1, \ldots, f_N)$ and D corresponds to the set of finite linear combinations of finite linear combinations of functions $\phi_1(m_1)\phi_2(m_2) \cdots \phi_N(m_N)$ such that $f_k^{n_k}\phi_k \in L^2(M_k, d\mu_k)$.

To prove essential self-adjointness we use Proposition 2 of Section VIII.3. First, since μ_k is finite and $f_k^{n_k} \in L^p(M_k, d\mu_k)$ we conclude that $f_k^l \in L^p(M_k, d\mu_k)$ for $1 \leq p < \infty$. From this it follows immediately that $P(f_1, \ldots, f_N)$ is in L^p for all such p; in particular $P(f_1, \ldots, f_N) \in L^4(\bigtimes_{k=1}^N M_k, \otimes_{k=1}^N d\mu_k)$. Since $f_k^{n_k}$ is self-adjoint on D_k, D_k contains the characteristic functions of measurable sets in M_k. Thus D contains all finite linear combinations of the characteristic functions of rectangles. The remarks on product measures at the end of Section I.4 show that the characteristic function of any measurable set in $\bigtimes_{k=1}^N M_k$ is equal to such a finite linear combination except on a set of arbitrarily small $\otimes_{k=1}^N d\mu_k$ measure. Thus the simple functions on $\bigtimes_{k=1}^N M_k$ can be approximated in the L^p sense ($1 \leq p < \infty$) by elements of D. In particular D is dense in $L^4(\bigtimes_{k=1}^N M_k, \otimes_{k=1}^N d\mu_k)$. Essential self-adjointness now follows from Proposition 2.

To show that P is essentially self-adjoint on D^e we need only show (by Problem 14) that $\overline{P \restriction D^e}$ extends $P \restriction D$. Suppose $\otimes_{k=1}^N \phi_k \in D$. Then $\phi_k \in D(A_k^{n_k})$, so since D_k^e is a domain of essential self-adjointness of $A_k^{n_k}$ there is a sequence $\{\phi_k^\ell\}_{\ell=1}^\infty$ so that $\phi_k^\ell \to \phi_k$, and $A_k^{n_k}\phi_k^\ell \to A_k^{n_k}\phi_k$. An easy estimate shows that this implies that $A_k^m \phi_k^\ell \to A_k^m \phi_k$ for all $1 \leq m \leq n_k$. Therefore $\otimes_{k=1}^N \phi_k^\ell \to \otimes_{k=1}^N \phi_k$ and $P(A_1, \ldots, A_N)(\otimes_{k=1}^N \phi_k^\ell) \to P(A_1, \ldots, A_N)(\otimes_{k=1}^N \phi_k)$. The same argument works for finite linear combinations of vectors of the form $\otimes_{k=1}^N \phi_k$ so $\overline{P \restriction D^e}$ extends $P \restriction D$. This completes the proof of (a).

To prove (b), suppose that $\lambda \in \overline{P(\sigma(A_1), \ldots, \sigma(A_N))}$. If I is any open interval about λ then $P^{-1}(I)$ contains a product $\bigtimes_{k=1}^N I_k$ of open intervals so that $I_k \cap \sigma(A_k) \neq \phi$. Since $\sigma(A_k) = \text{ess range} f_k^{n_k}$, $\mu_k[(f_k^{n_k})^{-1}(I_k)] \neq 0$ so

$$\mu[P(f_1, \ldots, f_N)^{-1}(I)] \neq 0.$$

That is, $\lambda \in \text{ess range } P(f_1, \ldots, f_N)$ which equals $\sigma(\overline{P(A_1, \ldots, A_N)})$ by the first proposition in Section VIII.3. Conversely if $\lambda \notin \overline{P(\sigma(A_1), \ldots, \sigma(A_N))}$ then $(\lambda - P(f_1, \ldots, f_N))^{-1}$ is bounded a.e. on $\bigtimes_{k=1}^N M_k$ so $\lambda \in \rho(\overline{P(A_1, \ldots, A_N)})$. ∎

If $A_1, \ldots, A_N$ are bounded, $P(\sigma(A_1), \ldots, \sigma(A_n))$ is closed, but in general it is not (Problem 43). The following corollary displays the two most important special case of Theorem VIII.33.

Corollary Let $A_1, \ldots, A_N$ be self-adjoint operators on $\mathscr{H}_1, \ldots, \mathscr{H}_N$ and suppose that, for each k, D_k is a domain of essential self-adjointness for A_k. Then,

(a) The operators $A_\pi = A_1 \otimes \cdots \otimes A_N$ and $A_\Sigma = A_1 + \cdots + A_N$ are essentially self-adjoint on $D = \otimes_{k=1}^N D_k$.

(b) $\sigma(A_\pi) = \overline{\prod_{k=1}^N \sigma(A_k)}$ and $\sigma(A_\Sigma) = \overline{\sum_{k=1}^N \sigma(A_k)}$.

Example 1 Suppose that $V(x)$ is a potential so that $H_1 = -\Delta_x + V(x)$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R}^3)$. Then $H_2 = -\Delta_x + V(x) + -\Delta_y + V(y)$ is essentially self-adjoint on the set of finite sums of products $\phi(x)\psi(y)$, with $\phi, \psi \in \mathscr{S}(\mathbb{R}^3)$. Further $\sigma(H_2) = \overline{\sigma(H_1) + \sigma(H_1)}$.

Example 2 (second quantization of the free Hamiltonian) Let $\mathscr{H}$ be a Hilbert space, $\mathscr{F}(\mathscr{H})$ the associated Fock space over $\mathscr{H}$ (see Section II.4). Suppose that A is a self-adjoint operator on $\mathscr{H}$ with a domain of essential self-adjointness D. Corresponding to each such A we can define an operator $d\Gamma(A)$ on $\mathscr{F}(\mathscr{H})$ as follows. Let $A^{(n)} = A \otimes I \cdots \otimes I + I \otimes A \otimes \cdots \otimes I \cdots + I \otimes \cdots \otimes A$ on $\otimes_{k=1}^n D$. Let $D_A \subset \mathscr{F}(\mathscr{H})$ be the set of $\psi = \{\psi_0, \psi_1, \ldots\}$ such that $\psi_n = 0$ for n large enough and $\psi_n \in \otimes_{k=1}^n D$ for each n. D_A is dense in $\mathscr{F}(\mathscr{H})$ since D is dense in $\mathscr{H}$. Define $A^{(0)} = 0$ and $d\Gamma(A) = \sum_{n=0}^{\infty} A^{(n)}$. $d\Gamma(A)$ makes sense on D_A and easily seen to be symmetric. By Theorem VIII.33, $A^{(n)}$ is essentially self-adjoint on $\otimes_{k=1}^n D$. Thus $A^{(n)} + \mu i$ has a dense range on $\otimes_{k=1}^n D$ whenever $\mu \in \mathbb{R}$ and $\mu \neq 0$. From this it follows quickly that $d\Gamma(A) \pm i$ has a dense range on D_A. Thus $d\Gamma(A)$ is essentially self-adjoint on D_A. If A is the quantum mechanical operator which corresponds to the free energy, $d\Gamma(A)$ is called the *second quantization* of the free energy. $d\Gamma(A)$ commutes with the projections onto the symmetric and antisymmetric Fock spaces and it follows that $d\Gamma(A) \upharpoonright \mathscr{F}_s(\mathscr{H})$ and $d\Gamma(A) \upharpoonright \mathscr{F}_a(\mathscr{H})$ are essentially self-adjoint on $D \cap \mathscr{F}_s(\mathscr{H})$ and $D \cap \mathscr{F}_a(\mathscr{H})$ respectively.

Part (b) of Theorem VIII.33 holds when $A_1, \ldots, A_N$ are allowed to be arbitrary bounded operators. Because of the techniques involved, we delay the proof until Chapter XIII, where we will also discuss some cases where $A_1, \ldots, A_N$ are unbounded but not self-adjoint.

VIII.11 Three mathematical problems in quantum mechanics

Our purpose in this short section is to describe briefly the mathematical model of quantum mechanics and to describe three general mathematical problems which arise. In the Notes we discuss how the model can be "derived" from various axiomatic schemes.

Quantum mechanical systems are described by operators and vectors in a separable Hilbert space $\mathscr{H}$. Corresponding to every vector of norm one in $\mathscr{H}$ there is a physical state. Two such vectors correspond to the same state

if and only if they differ by a complex multiple of absolute value one. Corresponding to each observable, there is a self-adjoint operator A on $\mathscr{H}$. If the system is in the state φ and we measure the observable corresponding to A, the probability distribution of the value of the measurement is $d(\varphi, P_\lambda \varphi)$ where P_Ω is the projection-valued measure associated to A. That is, the probability that the value of the measurement will lie in the interval $[a, b]$, $a, b \in \mathbb{R}$, is $(\varphi, P_{[a,b]}\varphi)$. The dynamics of the system is given by a continuous one-parameter group of unitary operators $U(t)$. If the system is in the state φ at time $t = 0$, then it is in the state $U(t_0)\varphi$ at time $t = t_0$. For most systems, there is a particularly useful realization of $\mathscr{H}$ as $L^2(M, d\mu)$ and a simple correspondence between classical observables and their quantum-mechanical counterparts, self-adjoint operators on $L^2(M, \mu)$ (see the example).

The self-adjoint generator H of the group $U(t)$ is of special interest. It is called the Hamiltonian and is the operator corresponding to the classical energy observable. For vectors $\varphi \in D(H)$ we have

$$\frac{d}{dt}[U(t)\varphi] = iH[U(t)\varphi]$$

which is called the Schrödinger equation. The point spectrum of H is of interest because the corresponding eigenfunctions are stationary states of the system; the typical reaction of the system to outside stimuli is to move from one stationary state to another emitting light whose frequency is proportional to the difference between the corresponding point spectra.

There are three general mathematical problems which arise in any quantum mechanical model:

(1) *Self-adjointness*: In most cases, physical reasoning gives a formal expression for the Hamiltonian and other observables as operators on a realization of $\mathscr{H}$ as $L^2(M, d\mu)$. We use the word "formal" because domains are not specified. It is usually easy to find a domain on which a given formal expression is a well-defined symmetric operator. The first mathematical problem is to prove essential self-adjointness or, if the operator is not essentially self-adjoint, to investigate the various self-adjoint extensions and choose the "right one" to be the observable.

(2) *Spectral analysis*: The second problem is to investigate the spectra of the observables (in particular, the Hamiltonian) and to estimate the position and multiplicity of the point spectra.

(3) *Scattering theory*: The third problem is to describe in some way the behavior of the system for large t.

The development and application of techniques for resolving these problems occupies much of Volumes II–IV. Self-adjointness is studied in Chapter X, spectral analysis in Chapters XII and XIII, and scattering theory in Chapter XI.

We do not mean to imply that all interesting mathematical problems associated with quantum mechanics fall under one of these three headings, far from it. But, these three problems are central to a rigorous mathematical description of quantum mechanics.

Example (n-electron atom) We will very briefly describe an approximate model for the n-electron atom. The classical energy of the n electrons is

$$h = \sum_{k=1}^{n} \frac{(p_x^k)^2 + (p_y^k)^2 + (p_z^k)^2}{2m} - \sum_{k=1}^{n} \frac{ne^2}{|r_k|} + \sum_{\substack{k,\ell=1 \\ k<\ell}}^{n} \frac{e^2}{|r_k - r_\ell|}$$

where p_x^k, p_y^k, p_z^k are the x, y, and z components of the momentum of the kth electron, $r_k = \langle x_k, y_k, z_k \rangle$ its position, m and e its mass and charge. The term $-ne^2/|r_k|$ is the potential energy of the kth electron due to the attraction of the protons in the nucleus; the term $e^2/|r_k - r_\ell|$ is the contribution to the potential energy due to the repulsion between the kth and ℓth electrons.

We take as our Hilbert space $\mathscr{H} = L^2(\mathbb{R}^{3n})$ and make the following correspondence between the classical observables and operators on $\mathscr{H}$ (we choose units in which the rationalized Planck's constant $\hbar$, is equal to one):

$$p_x^k \to \frac{1}{i}\frac{\partial}{\partial x_k} \qquad p_y^k \to \frac{1}{i}\frac{\partial}{\partial y_k} \qquad p_z^k \to \frac{1}{i}\frac{\partial}{\partial z_k}$$

x_k, y_k, z_k correspond to multiplication by x_k, y_k, z_k respectively,

$$h \to H = -\sum_{k=1}^{m} \frac{1}{2m} \Delta_k + V(r_1, \ldots, r_k)$$

where

$$\Delta_k = \frac{\partial^2}{\partial x_k^2} + \frac{\partial^2}{\partial y_k^2} + \frac{\partial^2}{\partial z_k^2}$$

and V denotes the operator which acts by multiplication by the function

$$-\sum_{k=1}^{n} \frac{ne^2}{|r_k|} + \sum_{k<\ell}^{n} \frac{e^2}{|r_k - r_\ell|}$$

All of the operators are essentially self-adjoint on $\mathscr{S}(\mathbb{R}^{3n})$, though the proof in the case of H is not at all immediate (see Section X.2). The dynamics is

given by the unitary group $U(t) = e^{-itH}$. If $\varphi \in \mathscr{H}$, $\|\varphi\| = 1$, is the state of the system at $t = 0$, then

$$\int_{x_k=a}^{b} \int_{\mathbb{R}^{3n-1}} |\varphi(x_1 \ldots, z_n)|^2 \, dx_1 \cdots dz_n$$

is the probability at $t = 0$, that the x coordinate of the kth particle will be in the interval (a, b) and

$$\int_{x_k=a}^{b} \int_{\mathbb{R}^{3n-1}} |(U(t_0)\varphi)(x_1, \ldots, z_n)|^2 \, dx_1 \cdots dz_n$$

is the probability at $t = t_0$. It is clear that the spectral analysis of H and the large t behavior of e^{-itH} are difficult mathematical problems.

We remark that this model is a rather crude approximation to the n-electron atom for several reasons: We have ignored electron spin and the Pauli exclusion principle. We have also ignored the motion of the nucleus, treating it as fixed. And finally, the model is nonrelativistic.

NOTES

Section VIII.1. The theory of unbounded operators was stimulated by attempts in the late 1920s to put quantum mechanics on a rigorous mathematical foundation. The systematic development of the theory is due to von Neumann, "Allgemeine Eigenwerttheorie Hermitescher Functionaloperatoren," *Math. Ann.* **102**, 49–131 (1929–1930) and M. Stone, "Linear Transformations in Hilbert Spaces and their Applications to Analysis," *Amer. Math. Soc. Colloq. Publ.* **15**, New York, 1932. The technique of using the graph to analyze unbounded operators was introduced by von Neumann in "Über Adjungierte Funktionaloperatoren," *Ann. Math.* (2) **33** (1936), 294–310.

A function on $[a, b] \subset \mathbb{R}$ is said to be *absolutely continuous* if, given $\varepsilon > 0$, there is a $\delta > 0$ so that

$$\sum_{k=1}^{n} |f(x_i') - f(x_i)| < \varepsilon$$

for every finite collection of disjoint intervals $[x_i, x_i']$ satisfying

$$\sum_{i=1}^{n} |x_i' - x_i| < \delta.$$

We then have the *Fundamental Theorem of Calculus*: If f is absolutely continuous on $[a, b]$, then f is differentiable a.e., $f'(x) \in L^1[a, b]$, and f is the indefinite integral of $f'(x)$. Conversely, if $g(x) \in L^1[a, b]$, then the indefinite integral, $G(x)$, of $g(x)$ is absolutely continuous and $G'(x) = g(x)$ a.e.

Section VIII.2. Theorem VIII.3 which is due to von Neumann (in the first paper cited above) is a special case of Theorem X.2 and its corollary. In his paper, von Neumann attributes the isolation of the notion of self-adjointness to E. Schmidt. We remark that von Neumann calls symmetric operators "Hermitian" and self-adjoint operators "hypermaximal Hermitian."

Section VIII.3. The fact that Hilbert's spectral resolution would not carry through for arbitrary symmetric operators was made clear by Carleman's book *Sur les équations intégrales singulières à noyau réel et symétrique*, Almquist and Wilesells, Uppsala, 1923. Von Neumann first discussed the spectral decomposition of unbounded operators in his investigation of the mathematical problems of quantum theory. The systematic proofs first appeared in the works of Von Neumann and Stone mentioned above and in F. Reisz, "Über die linearen Transformation des komplexen Hilbertschen Raumes," *Acta Sci. Math. (Szeged)* **5** (1930–1932), 23–54. Many of the ideas of spectral analysis already appear in matrix form in the work of A. Wintner.

One can develop a theory of integration with respect to vector-valued measures. This theory can then be applied to the projection-valued measure associated to any self-adjoint operator A. In particular, one can prove that for any $\varphi \in D(A)$,

$$A\varphi = \int \lambda \, d(P_\lambda \varphi)$$

where this integral converges strongly, that is, the Riemann–Stieltjes sums converge in norm to $A\varphi$. This is a stronger notion of convergence that we used in Section VIII.3 where the integral converged weakly.

Section VIII.4. Stone's theorem was announced in his paper "Linear Transformations in Hilbert Space, III," *Proc. Nat. Acad. Sci. U.S.A.* **15** (1929), 198–200, and was proved in "On One-Parameter Unitary Groups in Hilbert Space," *Ann. Math.* (2) **33** (1932), 643–648. Theorem VIII.9 appeared in von Neumann, "Über einen Satz von Herrn M. H. Stone," *Ann. Math.* (2) **33** (1932), 567–573. Our proof of Stone's theorem is due to Gårding and Wightmann (unpublished). The idea of using the group invariance to prove essential self-adjointness is due to Nelson, "Analytic Vectors," *Ann. Math.* **70** (1959), 572–614.

Let G be a locally compact Lie group and let $U(g)$ be a continuous unitary representation of G on $\mathscr{H}$, dg Haar measure on G. Then the set D of finite linear combinations of vectors of the form

$$\varphi_f = \int_G f(g)U(g)\varphi \, dg, \qquad \varphi \in \mathscr{H}, \quad f \in C_0^\infty(G)$$

is a dense set contained in the domains of the generators of all one-parameter subgroups of G and these generators take D into itself. This statement is due to L. Gårding, "Notes on Continuous Representations of Lie Groups," *Proc. Nat. Acad. Sci. U.S.A.* **33** (1947), 331–332 and D is often called the "Gårding domain." The existence of the Gårding domain is important because it allows one to get a representation of the Lie algebra of G on D.

Section VIII.5. The example due to Nelson is unpublished but a similar example appears in the "Analytic Vectors" paper cited above. Nelson also proves that if A and B are symmetric, D a dense set contained in $D(A) \cap D(B)$ and invariant under A and B, $AB\varphi - BA\varphi = 0$ for $\varphi \in D$, *and* $A^2 + B^2$ is essentially self-adjoint on D, then A and B are essentially

self-adjoint on D and their closures commute. The original proof of Theorem VIII.14 may be found in J. von Neumann, "Die Eindeutigkeit der Schrödingerschen Operatoren," *Math. Ann.* **104** (1931), 570–578. A more modern proof can be found in Kastler, "The C^*-Algebra of a Free Boson Field, I," *Commun. Math. Phys.* **I** (1965), 14–48. The Weyl relations were introduced in H. Weyl, "Quantenmechanik und Gruppentheorie," *Z. Phys.* **46** (1927), 1–46. We prove Theorem VIII.14 in Chapter XIV (see also Problem 30 in Chapter X).

Concerning the question of a converse to the corollary to Theorem VIII.14 it is known that if P and Q are symmetric on D and (a) and (b) hold *and* $P^2 + Q^2$ is essentially self-adjoint on D, then P and Q are essentially self-adjoint on D and the groups satisfy the Weyl relations. For a proof and a discussion of the generalization to n degrees of freedom see J. Dixmier, "Sur la Relation $i(PQ - QP) = I$," *Compos. Math.* **13** (1956), 263–269. Also of interest is B. Fuglede, "On the Relation $PQ - QP = iI$," *Math. Scand.* **20** (1967), 79–88.

Section VIII.6. The spectral theory for bounded operators was originally expressed in terms of quadratic forms. It is an interesting historical fact that the simple properties of quadratic forms which are semibounded were not really appreciated until twenty-five years after the spectral theory had been extended to unbounded objects by using operators instead of forms. The idea of the relations of forms and operators is implicit in the work of Friedrichs discussed in the notes to Section X.3 (especially in Freudenthal's proof) but the Friedrichs extension theorem was always expressed in terms of operators before 1950. In the 1950s, Theorems VIII.15 and VIII.16 were independently discussed and discovered by a variety of authors: particularly by P. Lax and A. Milgram in "Parabolic Equations," *Ann. Math. Study* **33** (1954), 167–190; T. Kato in "Quadratic forms in Hilbert spaces and asymptotatic perturbation series," Tech. Rep. No. 9, Univ. of Calif. (1955), and by J. Lions in his work *Équations différentielles opérationnelles et problèmes aux limites*, Springer, New York, 1961. The discussion and proof of Theorem VIII.15 in terms of scales of spaces was emphasized by Nelson, see, e.g. E. Nelson, *Topics in Dynamics*, Vol. I, Princeton Univ. Press, Princeton, New Jersey, 1970 for additional discussion. There is also an exhaustive study of quadratic forms in Chapter 6 of T. Kato, *Perturbation for Linear Operators*, Springer–Verlag, Berlin and New York, 1966, and a nice discussion in Chapter 12 of M. Schechter, *Principles of Functional Analysis*, Academic Press, New York, and London 1971.

The term "accretive" originally appeared in K. Friedrichs "Symmetric Positive Linear Differential Equations," *Comm. Pure. Appl. Math.* **11** (1958), 333–418 as something of a joke, but it caught on. It referred to operators with $\mathrm{Re}(u, Au) \geq 0$ for all $u \in D(A)$. The study of the such operators was essentially initiated by R. S. Phillips in "Perturbation Theory for Semigroups of Linear Operators," *Trans. Amer. Math. Soc.* **74** (1954), 199–221 (Phillips studied dissipative operators, that is, operators A with $\mathrm{Re}(u, Au) \leq 0$ for all $u \in D(A)$). Sectorial was then used if $\{(u, Au)\} \subset \{z \,|\, |\arg(z - w)| < \theta\}$ for some w and some $\theta < \pi/2$. These definitions are often carried over to the forms, that is, what we have called strictly accretive is often called sectorial. Since rotated as well as translated sectors often arise in applications, we have introduced the term "strictly accretive" and extended the notion of "sectorial."

m-accretive operators are maximal accretive operators in the same sense that self-adjoint operators are maximal symmetric operators. We return to this question in Section X.6.

Section VIII.7. For much of this section, the reader can consult Kato's book cited above for additional discussion.

The notion of norm resolvent convergence is the restriction to self-adjoint operators of a natural topology on closed operators from one Banach space to another. Krein and coworkers introduced a natural metric on closed subspaces of a Banach space in the 1940s. Explicitly, given M and N in a Banach space X, one defines

$$d(M, N) = \sup_{u \in M, \|u\| = 1} \left(\inf_{v \in N, \|v\| = 1} \|u - v\| \right)$$

Then $M \subset N$ if and only if $d(M, N) = 0$. If $\hat{d}(M, N) = \max[d(M, N), d(N, M)]$, $\hat{d}$ is a metric on all closed subspaces. If $\Gamma(T)$ is the graph of T, one can introduce a metric on all closed operators from X to Y, by $\rho(T, S) = \hat{d}(\Gamma(T), \Gamma(S))$, where, say, $\|\langle x, y \rangle\|_{X \times Y} = \|x\|_X + \|y\|_Y$. This produces a topology on the closed operators first introduced by J. Newburgh in "A Topology for Closed Operators," *Ann. Math.* **53** (1951), 250–255. When restricted to the self-adjoint operators, this is precisely the topology of norm resolvent convergence.

Theorems VIII.21 and VIII.22 are stated most naturally in terms of the theory of semigroups of operators on an arbitrary Banach space. Theorem VIII.21 seems to have been first proven explicitly (in the general semigroup language) in H. Trotter, "Approximation of Semigroups of Operators" *Pacific J. Math.* **8** (1959), 887–919 although it was something of a folk theorem at the time. Theorem VIII.22 was also proven by Trotter in the above paper although one point in his proof was clarified by T. Kato in "Remarks onPseudo-Resolvents and Infinitesimal Generators of Semigroups," *Proc. Jap. Acad.* **35** (1959), 467–468. Theorem VIII.21 is sometimes called the Trotter–Kato theorem also. For a discussion of norm and strong convergence of operators which are not necessarily self-adjoint, see Kato's book: Section IV.2 (norm), Sections VIII.1 and VIII.3 (strong).

Theorems like Theorems VIII.23 and VIII.24 were first proven in F. Rellich, "Störungstheorie der Spektralzerlegung, II," *Math. Ann.* **113** (1936), 667–685. Extensions of Rellichs' results appear in Sz.-Nagy "Perturbations des transformations autoadjointes dans l'espace de Hilbert," *Comm. Math. Helv.* **19** (1946–1947), 347–366; and E. Heinz, "Beiträge zur Störungstheorie der Spektralzerlegung," *Math. Ann.* **123** (1951), 415–438.

The systematic study of graph limits was begun in J. Glimm and A. Jaffe, "Singular Perturbations of Self-Adjoint Operators," *Comm. Pure Appl. Math.* **22** (1969), 401–414. We return to their ideas in Section X.10.

Section VIII.8. The extension of Lie's theorem to infinite dimensional cases was first made by H. Trotter, "On the Product of Semigroups of Operators," *Proc. Amer. Math. Soc.* **10** (1959), 545–551. He proved Theorem VIII.31 in the general context of semigroups on a Banach space. His proof was later simplified in P. R. Chernoff, "Note on Product Formulas for Operator Semigroups," *J. Func. Anal.* **2** (1968), 238–242.

The proof we give to Theorem VIII.30 is given in E. Nelson, "Feynman Integrals and the Schrödinger Equation," *J. Math. Phys.* **5** (1964), 332–343.

Extensions of Trotters formula to various special cases where $A + B$ is not essentially self-adjoint but has a definition as a sum of forms have been given by W. Faris, "The Product Formula for Semigroups Defined by Friedrichs Extensions," *Pacific J. Math.* **22** (1967), 47–70 and P. R. Chernoff, "Semigroup Product Formulas and Addition of Unbounded Operators," *Bull. Amer. Math. Soc.* **76** (1970), 395.

Section VIII.10. The first mathematical treatment of second quantization may be found in J. Cook, "The Mathematics of Second Quantization," *Trans. Amer. Math. Soc.* **74**, 222–245. For more information see I. Segal, "Tensor Algebras over Hilbert Spaces, I," *Trans. Amer. Math. Soc.* **81** (1956) 106–134.

The notation "$d\Gamma$" arises in the following way. $\mathscr{F}(\mathscr{H})$ is an algebra in a natural way with a product defined so that $(\psi_1 \otimes \cdots \otimes \psi_n) \cdot (\psi_{n+1} \otimes \cdots \otimes \psi_{n+k}) = \psi_1 \otimes \cdots \otimes \psi_{n+k}$. This product is denoted by $\otimes$. Thus $\psi \otimes \phi$ is defined for all $\psi, \phi \in \mathscr{F}(\mathscr{H})$. The natural "automorphisms" of $\mathscr{F}(\mathscr{H})$ are invertible linear, norm preserving maps, V, obeying $V(\psi \otimes \phi) = V\psi \otimes V\phi$. The natural automorphisms of $\mathscr{H}$ are just the unitaries. With each unitary, U, one can associate uniquely an automorphism, $\Gamma(U)$ on $\mathscr{F}(\mathscr{H})$ obeying $\Gamma(U) = U$ on $\mathscr{H}$ by requiring that on $\mathscr{H}^n = \otimes_{k=1}^n \mathscr{H}$, $\Gamma(U)$ be just $U \otimes \cdots \otimes U$ (n times). Thus Γ maps the group of unitaries on $\mathscr{H}$ into the group of automorphisms on $\mathscr{F}(\mathscr{H})$ in a strongly continuous manner. $d\Gamma$ is then defined by requiring $e^{it d\Gamma(A)} = \Gamma(e^{itA})$; that is for any self-adjoint A on $\mathscr{H}$, $d\Gamma(A)$ is the infinitesimal generator of the strongly continuous unitary group $\Gamma(e^{itA})$. In the language of Lie theory, $d\Gamma$ is differential of Γ as a map on the "Lie algebra" of the group of unitaries in $\mathscr{H}$ to the Lie algebra of the group of unitaries on $\mathscr{F}(\mathscr{H})$. That the $d\Gamma$ defined in the text has a closure equal to $d\Gamma$ as defined in the above paragraph is a simple exercise.

In the usual physicist's notation, if $\mathscr{H} = L^2(\mathbb{R}^3, dx)$ and A is defined by $(Af)(x) = \omega(x)f(x)$, then $d\Gamma(A)$ is what is written $\int \omega(x) a^*(x) a(x)\, dx$.

The proof of Theorem VIII.33 shows how the spectral theorem allows one to use L^p techniques on abstract Hilbert space problems. By using the spectral theorem one can often formulate the given problem in terms of $L^2(M, d\mu)$ for some convenient measure space $\langle M, \mu \rangle$. After this has been done the standard theorems and estimates of L^p theory can often be used.

Section VIII.11. Attempts at an a priori justification of the quantum mechanical picture we discuss go back to von Neumann's famous *Mathematische Grundlagen der Quantenmechanik*, Springer, New York, 1932 (reissued by Springer–Verlag, Berlin and New York, 1968; English transl. published by Princeton Univ. Press, Princeton, New Jersey, 1955). The approach of G. Mackey in *The Mathematical Foundations of Quantum Mechanics*, Benjamin, New York, 1963 and *Induced Representations of Groups and Quantum Mechanics*, Benjamin, New York, 1968 emphasizes the similarity with classical statistical mechanics and isolates the ad hoc elements of any axiomatic approach to quantum mechanics.

Maekey presents the following picture of classical statistical mechanics: The basic states of a classical mechanical system are points in a "phase space," M. Statistical states are just measures of total mass 1 on M. Observables are just measurable functions on M. Given a state μ and an observable f the measure $\nu_{\mu, f}$ on $\mathbb{R}$ given by $\nu_{\mu, f}(\Omega) = \mu(f^{-1}(\Omega))$ represents the probability a measurement of f, produces a value in Ω. The first remark of Mackey is that the points of M do not really enter in this picture; rather the family $\mathfrak{L}$ of Borel sets enter as the basic objects. The states μ are really functions on $\mathfrak{L}$ and to form $\nu_{\mu, f}$ one only needs f^{-1} which is a function from the Borel sets of $\mathbb{R}$ to $\mathfrak{L}$. The abstract structure on $\mathfrak{L}$ needed for $\nu_{\mu, f}$ to be a probability measure (total mass 1) on $\mathbb{R}$ is:

(i) $\mathfrak{L}$ has a partial order $\leq$ ($A \leq B$ if A is a subset of B) with a largest element, 1 (we have $M = 1$) and a smallest element 0 (we have $\varnothing = 0$).

(ii) $\mathfrak{L}$ has a complementation $'$ (A' is just the complement $M \setminus A$), with the basic properties $(A')' = A$; $A \leq B$ if and only if $B' \leq A'$; $1' = 0$.

(iii) $\mathfrak{L}$ is a countable lattice; that is, given $A_1, \ldots, A_n, \ldots \in \mathfrak{L}$ there exists

$$A = \bigvee_{n=1}^{\infty} A_n$$

with $A \geq A_n$ for all n and $A \leq B$ whenever $B \geq A_n$ for all n.

(iv) The lattice and complementation structures are related by $A \vee A' = 1$.

An abstract set $\mathfrak{L}$ with properties (i)–(iv) is called an **orthocomplemented lattice.** When one has such an object, $A, B \in \mathfrak{L}$ are called *disjoint* if $A \leq B'$. A *measure on* $\mathfrak{L}$ is a map $\mu: \mathfrak{L} \to \mathbb{R}^+ = \{a \in \mathbb{R} \mid a \geq 0\}$ with $\mu(1) = 1$, and

$$\mu\left(\bigvee_{n=1}^{\infty} A_n\right) = \sum_{n=1}^{\infty} \mu(A_n)$$

if A_i and A_j are disjoint for all i and j. An $\mathfrak{L}$-*valued measure* is a map $P: \mathscr{B} \to \mathfrak{L}$ where $\mathscr{B}$ is the family of Borel sets of $\mathbb{R}$ obeying $P(\mathbb{R}) = 1$,

$$P\left(\bigcup_{i=1}^{\infty} A_i\right) = \bigvee_{i=1}^{\infty} A_i \qquad \text{and} \qquad P(\mathbb{R} \backslash A) = P(A').$$

Thus Mackey's description of classical statistical mechanics leads to an abstract notion of *statistical system* as an orthocomplemented lattice. The observables are then $\mathfrak{L}$-valued measures and the states are measures on $\mathfrak{L}$. Given a state μ and an observable θ the Borel measure $\nu_{\mu,\theta}(\Omega) = \mu(\theta(\Omega))$ on $\mathbb{R}$ is interpreted as the probability that a measurement of the observable θ in the state μ will yield a value in Ω.

In the first quoted Mackey reference, there is a description of a set of reasonable axioms for the notion of measurement in a statistical system which lead to this orthocomplemented lattice. To obtain quantum mechanics, one might add the *ad hoc postulate* to the basic lattice picture: $\mathfrak{L}$ is just the family, $\mathfrak{L}_{\mathscr{H}}$, of closed subspaces of a separable Hilbert space $\mathscr{H}$ with the operations: $A \leq B$ if and only if $A \subseteq B$; $A' = A^{\perp}$, and $\bigvee_{n=1}^{\infty} A_n = \sum_{n=1}^{\infty} A_n$; $1 = \mathscr{H}$; $0 = \{0\}$. One is thus left with the problem of trying to justify this ad hoc postulate. Important partial progress towards this result was obtained in C. Piron, "Axiomatique Quantique," *Helv. Phys. Acta* 37 439–468 (1964). See also the discussion in the Jauch monograph mentioned below.

Once one has the ad hoc postulate, one can determine the states and observables in a more explicit form. A. Gleason in "Measures on the Closed Subspaces of a Hilbert Space," *J. Math. Mech.* 6, 885–894 (1957) proved that every measure on $\mathfrak{L}_{\mathscr{H}}$ has the following form: Each subspace $A \in \mathfrak{L}_{\mathscr{H}}$ is naturally associated with an orthogonal projection P with Ran $P = A$. Gleason proved that every measure μ on $\mathfrak{L}_{\mathscr{H}}$ has $\mu(A) = \text{tr}\,(\rho P)$ where ρ is some positive trace class operator with tr $\rho = 1$. By Theorems VI.17 and VI.21, we can find an orthonormal basis, $\{\Phi_n\}_{n=1}^{\infty}$ and $\alpha_1, \ldots, \alpha_n, \ldots \geq 0$ with $\sum_{n=1}^{\infty} \alpha_n = 1$, so that $\rho = \sum_{n=1}^{\infty} \alpha_n(\Phi_n, \cdot)\Phi_n$. Thus, arbitrary states are just sums of *vector states*, $\mu(P) = (\Phi_n, P\Phi_n)$ (in the language of Section XIV.1, these vector states are just the extreme points of the family of all states). As a result, one may analyze all states by considering only vector states.

$\mathfrak{L}_{\mathscr{H}}$-valued measures are precisely projection valued measures! Thus, by the spectral theorem (Theorem VIII.6), an observable is naturally associated with a self-adjoint operator A. The probability of obtaining a value in Ω, if A is measured in the vector state ψ is just $(\psi, P_\Omega \psi)$ where P_Ω is the p.v.m. for A.

Thus we see how the basic static elements of the picture in SectionVIII.11 arise from the ad hoc postulate. The picture of the dynamics enters from the following analysis†:

(1) For each time t there should be a map α_t on the set of all states, so that α_t takes a state at time s into the state at time $s + t$. Since $\alpha_t \alpha_{-t} = \alpha_0 = I$, each α_t should be a bijection. Moreover $\alpha(\rho_1 + \rho_2)$ should be $\alpha(\rho_1) + \alpha(\rho_2)$.

† For further discussion of this picture, see B. Simon: "From Automorphism to Hamiltonian," pp. 305–326 in *Studies in Mathematical Physics* (E. H. Lieb, B. Simon, and A. S. Wightman, eds.). Princeton Univ. Press, Princeton, New Jersey, 1976.

(2) Because any state is a sum of vector states, we only need to know how α behaves on vector states. Vector states are uniquely determined by the property that they are extreme points, so α must take vector states into themselves since α is invertible. Thus, α is a map of unit rays (that is, families of vectors of the form $\{e^{i\theta}\psi | \theta \in [0, 2\pi]\}$) into themselves. It is not quite arbitrary since there are vector states $\rho_{\Phi_1}, \ldots, \rho_{\Phi_4}$ with

$$\tfrac{1}{2}\rho_{\Phi_1} + \tfrac{1}{2}\rho_{\Phi_2} = \tfrac{1}{2}\rho_{\Phi_3} + \tfrac{1}{2}\rho_{\Phi_4}$$

and it is necessary that

$$\tfrac{1}{2}\rho_{\alpha(\Phi_1)} + \tfrac{1}{2}\rho_{\alpha(\Phi_2)} = \tfrac{1}{2}\rho_{\alpha(\Phi_3)} + \tfrac{1}{2}\rho_{\alpha(\Phi_4)}$$

For example, if Φ_1 and Φ_2 are orthogonal and

$$\Phi_3 = 2^{-1/2}(\Phi_1 + \Phi_2) \qquad \Phi_4 = 2^{-1/2}(\Phi_1 - \Phi_2)$$

we can use the above to conclude $\alpha(\Phi_1)$ is orthogonal to $\alpha(\Phi_2)$. In general, one shows that a map on the rays yields an automorphism of all the states, if and only if $|(\alpha(\Phi_1), \alpha(\Phi_2))| = |(\Phi_1, \Phi_2)|$ for all unit rays Φ_1, Φ_2.

(3) An analysis of E. Wigner in *Group Theory and Its Applications to the Quantum Mechanics of Atomic Spectra*, Academic Press, New York, 1959 [see also V. Bargmann, "Note on Wigner's Theorem on Symmetry Operations," *J. Math. Phys.* 5, 862–868 (1964)] uses the analysis of (2) to prove that every automorphism of the rays is of the form $\alpha(\Phi) = U\Phi$ with U unitary or antiunitary. Up to an overall change of phase, $U \to e^{i\theta}U$, U is uniquely determined by α.

(4) Since $\alpha_t = (\alpha_{t/2})^2$, the U_t of (3) must be unitary. It is natural to suppose that $t \to \alpha_t(\rho)$ is continuous. By a theorem of V. Bargmann "On the Unitary Ray Representations of Continuous Groups," *Ann. Math.* 59, 1–46, (1954) and E. Wigner "Unitary Representations of the Inhomogeneous Lorentz Group," *Ann. Math.* 40, 149–204 (1939), it is possible to choose the phases left arbitrary in (3) so that U_t is strongly continuous in t.

(5) Since $\alpha_t \alpha_s = \alpha_{t+s}$ we can conclude $U_t U_s = \lambda(t, s)U_{t+s}$ where $|\lambda(t, s)| = 1$. (There is still some arbitrariness left in phases.) A further analysis of Bargmann and Wigner (see the references cited above) implies that $\lambda(t, s) = \mu(t + s)\mu(t)^{-1}\mu(s)^{-1}$ for some measurable function μ with $|\mu(t)| = 1$. Letting $V(t) = \mu(t)U(t)$ we obtain a strongly continuous one-parameter group of unitaries which can then be analyzed by Stone's theorem as discussed in the text.

There is one further element of the picture which one can justify on the basis of more basic assumptions: this is the particular realization of $\mathscr{H}$ as $L^2(\mathbb{R}^n)$ with $p = i^{-1}\partial/\partial x$ etc. and the free Hamiltonian given by $H_0 = -(2m)^{-1}\Delta$. The realization of $\mathscr{H}$ as $L^2(\mathbb{R}^n)$ is connected, of course, with von Neumann's theorem on the uniqueness of solutions of the canonical commutation relations (see Section VIII.5). On a more fundamental level, it is connected with Euclidean invariance (symmetry under spatial translation and rotation) and position operators: this is discussed in the second Mackey reference and in A. Wightman, "On the Localizability of Quantum Mechanical Systems," *Rev. Mod. Phys.* 34, 845–872. (1962). The fact that H_0 is $-(2m)^{-1}\Delta$ is connected with Gallilean invariance as discussed in the second Mackey reference, Bargmann's Ann. Math. article (above), E. Inönu and E. Wigner "Representations of the Galilei Group," *Nuovo Cimento* 9 (1952), 705–718 and C. Piron, "Sur le quantification du système de deux particles," *Helv. Phys. Acta.* 38 (1965), 104–108.

We have just discussed in detail one approach to quantum axiomatics. For additional discussion and other approaches, see G. Birkhoff and J. von Neumann, "The Logic of Quantum Mechanics," *Ann. Math.* 37 (1936), 823–843; G. Dahn, "Attempt of an Axiomatic

Foundation of Quantum Mechanics and More General Theories, IV," *Commun. Math. Phys.* **9** (1968), 192–211; E. B. Davies, "Quantum Stochastic Processes," *Commun. Math. Phys.* **15** (1969), 277–304; E. B. Davies and J. T. Lewis, "An Operational Approach to Quantum Probability," *Commun. Math. Phys.* **17** (1970), 239–260; C. M. Edwards, "The Operational Approach to Algebraic Quantum Theory, I," *Commun. Math. Phys.* **16** (1970), 207–230; J. Gunson, "On the Algebraic Structure of Quantum Mechanics," *Commun. Math. Phys.* **6** (1967), 262–285; K. E. Hellwig and K. Kraus, "Operations and Measurements, I, II," *Commun. Math. Phys.* **11** (1969), 214–220; **16** (1970), 142–147; J. Jauch, *Foundations of Quantum Mechanics*, Addison-Wesley, Reading, Massachusetts, 1968; P. Jordan, J. von Neumann, and E. Wigner "On the Algebraic Generalization of the Quantum Mechanical Formalism," *Ann. Math.* **35** (1934), 29–64; G. Ludwig, "Attempt at an Axiomatic Foundation of Quantum Mechanics and more General Theories, I–III," *Z. Phys.* **181** (1964), 223–260; *Commun. Math. Phys.* **4** (1967), 331–348; **9** (1968), 1–12; B. Mielnile, "Geometry of Quantum States," *Commun. Math. Phys.* **9** (1968), 55–80; R. J. Plymon, "A Modification of Piron's Axioms," *Helv. Phys. Acta* **41** (1968), 69–74; R. J. Plymon, "C^*-Algebras and Mackey's Axioms," *Commun. Math. Phys.* **8** (1968), 132–146; J. Pool, "Baer *-Semigroups and the Logic of Quantum Mechanics," *Commun. Math. Phys.* **9** (1968), 118–141; J. Pool, "Semimodularity and the Logic of Quantum Mechanics," *Commun. Math. Phys.* **9** (1968), 212–228; E. Prugovečki, *Quantum Mechanics in Hilbert Spaces*, Academic Press, New York, 1971; I. Segal, "Postulates for General Quantum Mechanics," *Ann. Math.* **48** (1947), 930–940; V. Varadarajan, *Geometry of Quantum Theory*, Van Nostrand-Reinhold, Princeton, New Jersey, 1968; H. Weyl, *The Theory of Groups and Quantum Mechanics*, Dover, New York, 1931; N. Zierler, "Axioms for Non-relativistic Quantum Mechanics," *Pacific J. Math.* **11** (1961), 1151–1169.

Despite the rather enormous literature on these "first level" foundations of quantum theory, there is no definitive theory of quantum axiomatics. Probably the most important result of the attempts to axiomatize quantum theory is the mathemetical "spin-off" that has resulted: the theory of unbounded self-adjoint operators, Jordan algebras, and the C^*-algebra approach to quantum theory (discussed in Chapters XIX and XX), all have their origin in attempts at quantum axiomatization.

PROBLEMS

1. Let $\{\varphi_n\}$ be an orthonormal basis for a Hilbert space $\mathscr{H}$ and let e_∞ be a vector in $\mathscr{H}$ which is not a finite linear combination of the φ_n. Let D be the set of finite linear combination of elements of $\{\varphi_n\}$ and e_∞, and on D define

$$T(be_\infty + \sum_{i=1}^{N} c_i \varphi_i) = be_\infty$$

Show that $\overline{\Gamma(T)}$ contains both $\langle e_\infty, e_\infty \rangle$ and $\langle e_\infty, 0 \rangle$ and thus is not the graph of a linear operator.

2. Let S be an operator from $D(S)$ to $\mathscr{H}$ which is injective. Consider the following additional statements about S:

(1) S is a closed operator.

(2) Ran S is dense.
(3) Ran S is closed.
(4) For some constant C and all $\psi \in D(S)$, $\|S\psi\| \geq C\|\psi\|$.

(a) Prove that (1)–(3) imply (4) (*Hint*: Apply the closed graph theorem to S^{-1}).
(b) Prove that (2)–(4) imply (1)
(c) Prove that (1) and (4) imply (3)

Remark. Let T be a closed operator. Applying (a) to $\lambda - T$ we see that $\lambda \in \rho(T)$ if and only if $\lambda - T$ is bijective. (b) also has a "translation" of this sort.

†3. Prove that the operators in Example 5 of Section VIII.1 are closed.

4. (a) Suppose that C is a symmetric operator, $C \supset A$ and that $\text{Ran}(A + i) = \text{Ran}(C + i)$. Prove that $C = A$.
(b) Suppose that A is a symmetric operator with $\text{Ran}(A + i) = \mathscr{H}$ but $\text{Ran}(A - i) \neq \mathscr{H}$. Prove that A has no self-adjoint extensions.

5. Let $\mathscr{H} = \ell_2$. Let $D(A) = \{a \in \mathscr{H} \mid$ for some $N, \sum_{m=0}^{N} a_n = 0$ and $a_n = 0$ if $n > N\}$. For $a \in D(A)$, define $Aa \in \mathscr{H}$ by

$$(Aa)_n = i\left[\sum_{m=0}^{n-1} a_m + \sum_{m=0}^{n} a_m\right]$$

(a) Prove that $D(A)$ is dense in $\mathscr{H}$.
(b) Prove that A is symmetric. *Hint*: if $\sum_{m=0}^{N} a_n = 0$, then

$$(Aa)_n = i\left[\sum_{m=0}^{n-1} a_m - \sum_{m=n+1}^{N} a_m\right]$$

(c) Prove that $\text{Ran}(A + i)$ is dense in ℓ_2.
(d) Prove that $(1, 0, 0, \ldots) \in D(A^*)$ and that $(A^* + i)(1, 0, 0, \ldots) = 0$
(e) Prove that A has no self-adjoint extensions. (*Hint*: Apply Problem 4b to $\bar{A}$).

†6. Prove that the operator T in the example of Section VIII.2 is closed.

†7. Prove that the operators T_α in the example of Section VIII.2 are self-adjoint. (*Hint*: It follows from what was already proven that $\psi \in D(T_\alpha^*)$ implies that $\psi \in AC[0, 1]$ and $T_\alpha^* \psi = i\, d\psi/dx$.)

8. Consider $T = -d^2/dx^2$ as an operator on $L^2[\mathbb{R}]$ with domain $C_0^\infty(\mathbb{R})$. What is the adjoint of T? Is T essentially self-adjoint?

9. Consider $T = i\, d/dx$ as an operator on $L^2(0, \infty)$ with domain $C_0^\infty[0, \infty]$, the infinitely differentiable functions with compact support away from the origin. Is T essentially self-adjoint?

10. Suppose that A is a densely defined symmetric operator which is positive, that is, $(\varphi, A\varphi) \geq 0$ if $\varphi \in D(A)$.
(a) Prove that $\|(A + I)\varphi\|^2 \geq \|\varphi\|^2 + \|A\varphi\|^2$.
(b) Show that $\text{Ran}(A + I)$ is closed if A is a closed operator.
(c) Prove that A is essentially self-adjoint if and only if the equation $A^*\psi = -\psi$ has no nonzero solutions.

†11. Prove part (c) of Theorem VIII.7.

41. Let H_0 and V be closed, positive quadratic forms and let $\beta \in \mathbb{C}\backslash(-\infty, 0]$. Suppose that $Q(H_0) \cap Q(V)$ is dense in $\mathscr{H}$. Prove that $H_0 + \beta V$ defined as a quadratic form on $Q(H_0) \cap Q(V)$ is closed and sectorial.

42. Let T be a self-adjoint densely defined operator on a Hilbert space $\mathscr{H}$. Suppose that for some $\lambda_0 \in \rho(T)$, $R_{\lambda_0}(T)$ is a compact operator. Prove that $R_\lambda(T)$ is compact for all $\lambda \in \rho(T)$ and discuss the various kinds of spectra that T can have.

Remark. We study operators with compact resolvent in Chapter XIII.

43. (a) Give an example to show that the *closure* of the range of P on $\mathbf{X}_{k=1}^{n} \sigma(A_k)$ may be needed to obtain the whole spectrum of $P(A_1, \ldots, A_N)$.
(b) Prove that if $A_1, \ldots, A_N$ are bounded then the closure is *not* necessary.

44. Prove the uniqueness statement of Theorem VIII.32.

45. Let T be a closed operator. Prove that $M = \{\psi \mid \psi \in D(T), T\psi \in D(T^*)\}$ is dense and that T^*T defined on M is self-adjoint (*Hint*: Let S be the operator constructed in Theorem VIII. 32. Show that $D(S) \subset M$ and that T^*T is a symmetric extension of S).

46. Let T be a closed operator on a Hilbert space. Define, $N(T)$, the numerical range of T by $N(T) = \{\overline{(\psi, T\psi)} \mid \psi \in D(T): \|\psi\| = 1\}$.
(a) Prove $\sigma(T) \subset N(T) \cup N(T^*)^*$ where $N(T^*)^*$ is the set $\{\overline{(\psi, T^*\psi)} \mid \psi \in D(T)\}$.
(b) Find a T with $\sigma(T) \not\subset N(T)$ and thus with $N(T) \neq N(T^*)^*$. (*Hint*: Take T symmetric!)

47. Let A be self-adjoint on $D(A)$ in $\mathscr{H}_1$ and B be self-adjoint on $D(B)$ in $\mathscr{H}_2$. Use Theorem VIII.10 to prove that $A \otimes I + I \otimes B$ is essentially self-adjoint on $D(A) \otimes D(B)$. (*Hint*: $e^{itA} \otimes e^{itB}$ leaves $D(A) \otimes D(B)$ invariant.)

48. Let A be a closed symmetric operator with $A \neq A^*$. Let a and b be the quadratic forms with

$$Q(a) = D(A) \qquad a(\psi, \varphi) = (A\psi, A\varphi)$$
$$Q(b) = D(A^*) \qquad b(\psi, \varphi) = (A^*\psi, A^*\varphi)$$

Show that $a \subset b$ but $a \neq b$ despite the fact that a and b are positive symmetric forms.

49. A self-adjoint operator, A, is said to have **purely discrete spectrum** in (a, b) if $(a, b) \cap \sigma(A) = (a, b) \cap \sigma_{\text{disc}}(A)$.
(a) Prove that A has purely discrete spectrum in (a, b) if and only if $P_{(a+\varepsilon, b-\varepsilon)}$ is compact for all small ε where $\{P_\Omega\}$ is the family of spectral projections for A.
(b) Prove that A has purely discrete spectrum in (a, b) if and only if $f(A)$ is compact for every C^∞ function f with $\operatorname{supp} f \subset (a, b)$. (*Hint*: Use Problem 45 of Chapter VI.)
(c) Let $A_n \to A$ in the norm resolvent sense. Suppose that each A_n has purely discrete spectra in (a, b). Prove that A has purely discrete spectra in (a, b).

50. Let A be a positive self-adjoint operator
(a) Prove that $\|(A + w)^{-1}\| \leq w^{-1}$ for $w > 0$
(b) Prove that

$$\int_0^\infty w^{-\frac{1}{2}}(A + w)^{-1}\varphi \, dw$$

exists for all $\varphi \in \operatorname{Ran} A$.

(c) Prove that

$$A^{+1/2}\psi = \left[\frac{1}{\pi}\int_0^\infty w^{-1/2}(A+w)^{-1}\,dw\right] A\psi \qquad \text{for any} \quad \psi \in D(A).$$

(d) In the same way prove that

$$A^{\alpha}\psi = \frac{\sin \pi\alpha}{\pi}\int_0^\infty \left[w^{\alpha-1}(A+w)^{-1}\,dw\right] A\psi \quad \text{for any} \quad \psi \in D(A),$$

if $0 < \alpha < 1$.

(e) Prove that

$$\left(\lim_{\alpha \downarrow 0} \frac{A^{\alpha}-1}{\alpha}\right)\psi = (\log A)\psi \qquad \text{for any} \quad \psi \in D(A)$$

51. If A and B are self-adjoint operators with $A, B \geq 0$, we say $A \geq B$ if $Q(B) \supset Q(A)$ and $\langle \psi, B\psi\rangle \leq \langle \psi, A\psi\rangle$, for all $\psi \in D(A)$.

(a) If $0 \leq A \leq B$, prove that $A(A+w)^{-1} \leq B(B+w)^{-1}$ if $w \geq 0$.

(b) Prove that $A^{\alpha} \leq B^{\alpha}$ if $A \leq B$ and $0 < \alpha < 1$.

(c) Prove that $\log A \leq \log B$ if $A \leq B$.

**52.* Extend the proof of the spectral theorem in Problem 32 of Chapter VII to the unbounded case by using the polar decomposition for closed operators. Be sure to check that you can prove the polar decomposition without using the spectral theorem in the unbounded case. (*Hint*: You will need Problem 50).

Reference for Problem 52: Kato's book, pp. 281–282, 322–324, 334–335.

†*12.* Prove Theorem VIII.11 directly without using Theorem VIII.10.

13. Find two dense, linear subspaces of $L^2(\mathbb{R})$, D_1 and D_2, with $D_1 \cap D_2 = \{0\}$, so that x is essentially self-adjoint on D_1 and x^2 is essentially self-adjoint on D_2.

†*14.* Let A be a symmetric operator with domain $D \subset \mathscr{H}$. Let $D_1 \subset D$ be a dense linear subset of $\mathscr{H}$ and suppose that $A \upharpoonright D_1$ is essentially self-adjoint. Prove that A is essentially self-adjoint and $\bar{A} = \overline{A \upharpoonright D_1}$.

†*15.* (a) Prove that an operator A is closed if and only if its domain, $D(A)$, is complete under the norm

$$\|\psi\|_A = \|A\psi\| + \|\psi\|.$$

(b) Prove that a semibounded quadratic form is closed if and only if whenever

$$\varphi_n \in Q(q), \qquad \varphi_n \overset{\mathscr{H}}{\to} \varphi, \qquad \text{and} \qquad q(\varphi_n - \varphi_m, \varphi_n - \varphi_m) \underset{n,m\to\infty}{\to} 0,$$

then $\varphi \in Q(q)$ and $q(\varphi_n - \varphi, \varphi_n - \varphi) \to 0$.

†*16.* (a) Show that the quadratic form q associated with a semibounded self-adjoint operator A (Example 2 of Section VIII.6) is closed.
(b) Prove that any operator core for A is a form core for q.

†*17.* Prove the statements (a)–(d) in Example 3 of Section VIII.6.

†*18.* Fill in the details of Theorem VIII.16.

19. Let $A_n = (1 - 1/n)x$ on $L^2(\mathbb{R})$ and $A = x$. Show that one can choose domains of essential self-adjointness for A_n and A which have no nonzero vector in common but that $A_n \to A$ in the norm resolvent sense.

20. (a) Let $\{A_n\}$ and A be self-adjoint operators and suppose that for all $\varphi, \psi \in \mathscr{H}$ and all λ with $\operatorname{Im}\lambda \neq 0$, $(R_\lambda(A_n)\varphi, \psi) \to (R_\lambda(A)\varphi, \psi)$. Prove that $A_n \to A$ in the strong resolvent sense. (*Hint:* You will need the first resolvent fomula.)
(b) Let $\{A_n\}$ and A be self-adjoint operators. Use part (a) to prove that if $R_\lambda(A_n)$ converges strongly to $R_\lambda(A)$ in the lower half-plane then $R_\lambda(A_n)$ also converges strongly to $R_\lambda(A)$ in the upper half-plane.

†*21.* Extend the proofs of Theorems VIII.20 and VIII.21 to show that if $A_n \to A$ in the strong resolvent sense, then $e^{itA_n}\varphi \to e^{itA}\varphi$ *uniformly* for t in any finite interval.

†*22.* Fill in the details of the proofs of parts (b) and (c) of Theorem VIII.25.

23. (a) Let A_n be a sequence of self-adjoint operators and suppose that for each $\varphi \in \mathscr{H}$ and each $t \in \mathbb{R}$, $e^{itA_n}\varphi$ converges in $\mathscr{H}$. Prove that there exists a self-adjoint operator A so that $A_n \to A$ in the strong resolvent sense. (*Hint*: You will need to use von Neumann's theorem from Section VIII.4.)
(b) Give an example to show that the conclusion of (a) may not hold if e^{itA_n} converges weakly instead of strongly.

†*24.* Prove Theorem VIII.27b.

†*25.* Prove Theorem VIII.28.

26. Let $\{A_n\}$ be a uniformly bounded sequence of self-adjoint operators. Let A be a bounded self-adjoint operator. Prove that $A = \text{w.gr.-lim } A_n$ if and only if $A_n \to A$ in the weak operator topology.

27. Let $\{A_n\}$ and A be positive self-adjoint operators. Prove that $A_n \to A$ in the strong resolvent sense if and only if $(A_n + I)^{-1} \to (A + I)^{-1}$ strongly.

†28. Prove that if $\{A_n\}$ and A are uniformly bounded self-adjoint operators, then $A_n \to A$ in the strong resolvent sense if and only if $A_n \to A$ strongly.

29. Let A be self-adjoint.
(a) Prove that $tA \to t_0 A$ in the norm resolvent sense as $t \to t_0 \neq 0$.
(b) Prove that $e^{itA} \to e^{it_0 A}$ in norm if and only if A is bounded.

30.†(a) Prove that if $\{A_n\}$ and A are uniformly bounded self-adjoint operators and $A_n \xrightarrow{w} A$ but $A_n \not\xrightarrow{s} A$, then A_n does not converge to A in the weak resolvent sense.
(b) Where does the weak analogue of Theorem VIII.18 breakdown?

31. Is the form analogue of part (a) of Theorem VIII.25 true?

32. Prove that $A_n = nI$ has a strong graph limit as $n \to \infty$ which is not the graph of an operator.

33. Let $\{A_n\}$ be a *constant* sequence of symmetric operators (that is, $A_n = B$, $\forall n$). Show that the strong graph limit of the A_n is the closure of B.

34. Let R be the right shift operator on ℓ_2. Prove that the w.gr.-lim R^n is the zero operator while the st.gr.-lim R^n is the graph $\{\langle 0, 0\rangle\}$.

35. Prove directly (without using the Fourier transform) that $i^{-1}(d/dx)$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$.

†36. Prove the corollary to Theorem VIII.14.

†37. Fill in all the details of the proof of Theorem VIII.22.

38. (a) Let $\{A_n\}$ and A be positive self-adjoint operators and suppose that $e^{-tA_n} \to e^{-tA}$ strongly for each $t > 0$. Prove that $A_n \to A$ in the strong resolvent sense.
(b) Prove the analogue of (a) if strong convergence is replaced by norm convergence.

39. Let $U(t)$, $t \geq 0$, be a family of self-adjoint operators satisfying (i) $\|U(t)\| \leq e^{Et}$ for some $E \in \mathbb{R}$, (ii) $U(t)U(s) = U(t+s)$, (iii) the map $t \to U(t)$ is strongly continuous, (iv) $U(0) = I$. Then
(a) By mimicking our proof of Stone's theorem prove that $U(t) = e^{-At}$ for a unique self-adjoint operator A.
(b) Reach the same conclusion using the functional calculus.
(c) Prove that $A \geq -E$.

40. Let $\langle M, \mu\rangle$ be a measure space and $\mathscr{H} = L^2(M, d\mu)$. A map T of $L^2(M, d\mu)$ into itself will be called **positivity preserving** if $(Tf)(x) \geq 0$ a.e. whenever $f(x) \geq 0$ a.e. Let A, B be self-adjoint operators on $\mathscr{H}$ and suppose that e^{-tA} and e^{-tB} are positivity preserving for all $t \in \mathbb{R}$ and that $A + B$ is essentially self-adjoint on $D(A) \cap D(B)$. Prove that $e^{i(At+Bt)}$ is positivity preserving for each $t \in \mathbb{R}$.

The Fourier Transform

We have therefore the equation of condition

$$F(x) = \int dq\, Q \cos qx$$

If we substituted for Q any function of q, and conducted the integration from $q = 0$ to $q = \infty$, we should find a function of x: it is required to solve the inverse problem, that is to say, to ascertain what function of q, after being substituted for Q, gives as a result the function F(x), a remarkable problem whose solution demands attentive examination. *Joseph Fourier*

IX.1 The Fourier transform on $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{S}'(\mathbb{R}^n)$, convolutions

The Fourier transform is an important tool of both classical and modern analysis. We begin by defining it, and the inverse transform, on $\mathscr{S}(\mathbb{R}^n)$, the Schwartz space of C^∞ functions of rapid decrease.

Definition Suppose $f \in \mathscr{S}(\mathbb{R}^n)$. The **Fourier transform** of f is the function $\hat{f}$ given by

$$\hat{f}(\lambda) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ix\cdot\lambda} f(x)\, dx$$

where $x \cdot \lambda = \sum_{i=1}^n x_i \lambda_i$. The **inverse Fourier transform** of f, denoted by $\check{f}$, is the function

$$\check{f}(\lambda) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{ix\cdot\lambda} f(x)\, dx$$

We will occasionally write $\hat{f} = \mathscr{F}f$.

Since every function in Schwartz space is in $L^1(\mathbb{R}^n)$, the above integrals make sense. Many authors begin by discussing the Fourier transform on $L^1(\mathbb{R}^n)$. We start with Schwartz space for two reasons: First, the Fourier transform is a one-to-one map of Schwartz space onto itself (Theorem IX.1). This makes it particularly easy to talk about the inverse Fourier transform, which of course turns out to be the inverse map. That is, on Schwartz space, it is possible to deal with the transform and the inverse transform on an equal footing. Though this is also true for the Fourier transform on $L^2(\mathbb{R}^n)$ (see Theorem IX.6), it is not possible to define the Fourier transform on $L^2(\mathbb{R}^n)$ directly by the integral formula since $L^2(\mathbb{R}^n)$ functions may not be in $L^1(\mathbb{R}^n)$; a limiting procedure must be used. Secondly, once we know that the Fourier transform is a one-to-one, bounded map of $\mathscr{S}(\mathbb{R}^n)$ onto $\mathscr{S}(\mathbb{R}^n)$, we can easily extend it to $\mathscr{S}'(\mathbb{R}^n)$. It is this extension that is fundamental to the applications in Sections 5, 6, and 8.

We will use the standard multi-index notation. A multi-index

$$\alpha = \langle \alpha_1, \ldots, \alpha_n \rangle$$

is an n-tuple of nonnegative integers. The collection of all multi-indices will be denoted by I_+^n. The symbols $|\alpha|$, x^α, D^α, and x^2 are defined as follows:

$$|\alpha| = \sum_{i=1}^{n} \alpha_i$$

$$x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}$$

$$D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \cdots \partial x_n^{\alpha_n}}$$

$$x^2 = \sum_{i=1}^{n} x_i^2$$

In preparation for the proof that $\hat{}$ and $\check{}$ are inverses, we prove:

Lemma The maps $\hat{}$ and $\check{}$ are continuous linear transformations of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$. Furthermore, if α and β are multi-indices, then

$$((i\lambda)^\alpha D^\beta \hat{f})(\lambda) = \widehat{D^\alpha((-ix)^\beta f(x))} \tag{IX.1}$$

Proof The map $\hat{}$ is clearly linear. Since

$$\begin{aligned}(\lambda^\alpha D^\beta \hat{f})(\lambda) &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \lambda^\alpha (-ix)^\beta e^{-i\lambda\cdot x} f(x)\, dx \\ &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \frac{1}{(-i)^\alpha} (D_x^\alpha e^{-i\lambda\cdot x})(-ix)^\beta f(x)\, dx \\ &= \frac{(-i)^\alpha}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\lambda\cdot x} D_x^\alpha ((-ix)^\beta f(x))\, dx\end{aligned}$$

We conclude that

$$\|\hat{f}\|_{\alpha,\beta} = \sup_{\lambda} |\lambda^{\alpha}(D^{\beta}\hat{f})(\lambda)| \leq \frac{1}{(2\pi)^{n/2}} \int |D_x^{\alpha}(x^{\beta}f)|\, dx < \infty$$

so $\hat{}$ takes $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$, and we have also proven (IX.1). Furthermore, if k is large enough, $\int (1+x^2)^{-k}\, dx < \infty$ so that

$$\|\hat{f}\|_{\alpha,\beta} \leq \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \frac{(1+x^2)^{-k}}{(1+x^2)^{-k}} |D_x^{\alpha}(-ix)^{\beta}f(x)|\, dx$$

$$\leq \frac{1}{(2\pi)^{n/2}} \left(\int (1+x^2)^{-k}\, dx \right) \sup_x \{(1+x^2)^{+k} |D_x^{\alpha}(-ix)^{\beta}f(x)|\}$$

Using Leibnitz's rule we easily conclude that there exist multi-indices α_j, β_j and constants c_j so that

$$\|\hat{f}\|_{\alpha,\beta} \leq \sum_{j=1}^{M} c_j \|f\|_{\alpha_j,\beta_j}$$

Thus, $\hat{}$ is bounded and by Theorem V.4 is therefore continuous. The proof for $\check{}$ is the same. ∎

We are now ready to prove the Fourier inversion theorem. The proof we give uses the original idea of Fourier.

Theorem IX.1 (Fourier inversion theorem) The Fourier transform is a linear bicontinuous bijection from $\mathscr{S}(\mathbb{R}^n)$ onto $\mathscr{S}(\mathbb{R}^n)$. Its inverse map is the inverse Fourier transform, i.e., $\check{\hat{f}} = f = \hat{\check{f}}$.

Proof We will prove that $\check{\hat{f}} = f$. The proof that $\hat{\check{f}} = f$ is similar. $\hat{\check{f}} = f$ implies that $\hat{}$ is surjective and $\check{\hat{f}} = f$ implies that $\hat{}$ is injective. Since $\hat{}$ and $\check{}$ are continuous maps of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$, it is sufficient to prove that $\check{\hat{f}} = f$ for f contained in the dense set $C_0^{\infty}(\mathbb{R}^n)$. Let C_ε be the cube of volume $(2/\varepsilon)^n$ centered at the origin in $\mathbb{R}^n$. Choose ε small enough so that the support of f is contained in C_ε. Let

$$K_\varepsilon = \{\mathbf{k} \in \mathbb{R} \mid \text{each } k_i/\pi\varepsilon \text{ is an integer}\}$$

Then

$$f(x) = \sum_{k \in K_\varepsilon} ((\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}, f)(\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}$$

is just the Fourier series of f which converges uniformly in C_ε to f since f is continuously differentiable (Theorem II.8). Thus

$$f(x) = \sum_{k \in K_\varepsilon} \frac{\hat{f}(k) e^{ik\cdot x}}{(2\pi)^{n/2}} (\pi\varepsilon)^n \tag{IX.2}$$

Since $\mathbb{R}^n$ is the disjoint union of the cubes of volume $(\pi\varepsilon)^n$ centered about the points in K_ε, the right-hand side of (IX.2) is just a Riemann sum for the integral of the function $\hat{f}(k)e^{ik\cdot x}/(2\pi)^{n/2}$. By the lemma, $\hat{f}(k)e^{ik\cdot x} \in \mathscr{S}(\mathbb{R}^n)$, so the Riemann sums converge to the integral. Thus $\check{\hat{f}} = f$. ∎

Corollary Suppose $f \in \mathscr{S}(\mathbb{R}^n)$. Then

$$\int_{\mathbb{R}^n} |f(x)|^2\, dx = \int_{\mathbb{R}^n} |\hat{f}(k)|^2\, dk$$

Proof This is really a corollary of the proof rather than the statement of Theorem IX.1. If f has compact support, then for ε small enough,

$$f(x) = \sum_{k \in K_\varepsilon} ((\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x},\ f(x))(\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}$$

Since $\{(\frac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}\}_{k \in K_\varepsilon}$ is an orthonormal basis for $L^2(C_\varepsilon)$,

$$\begin{aligned}
\int_{\mathbb{R}^n} |f(x)|^2\, dx &= \int_{C_\varepsilon} |f(x)|^2\, dx \\
&= \sum_{k \in K_\varepsilon} |((\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x},\ f(x))|^2 \\
&= \sum_{k \in K_\varepsilon} |\hat{f}(k)|^2 (\pi\varepsilon)^n \\
&\xrightarrow[\varepsilon \to 0]{} \int_{\mathbb{R}^n} |\hat{f}(k)|^2\, dk
\end{aligned}$$

This proves the corollary for $f \in C_0^\infty$. Since $\hat{\ }$ and $\|\cdot\|_2$ are continuous on $\mathscr{S}$ and C_0^∞ is dense, the result holds for all of $\mathscr{S}$. ∎

Example 1 We compute the Fourier transform of $f(x) = e^{-\alpha x^2/2} \in \mathscr{S}(\mathbb{R})$ where $\alpha > 0$.

$$\begin{aligned}
\hat{f}(\lambda) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-\alpha x^2/2} e^{-i\lambda\cdot x}\, dx \\
&= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \sqrt{\frac{2}{\alpha}} \exp\left(-t^2 - it\lambda\sqrt{\frac{2}{\alpha}}\right) dt \\
&= \frac{e^{-\lambda^2/2\alpha}}{\sqrt{\alpha\pi}} \int_{\mathbb{R}} \exp -\left(t + i\frac{\lambda}{\sqrt{2\alpha}}\right)^2 dt \\
&= \frac{e^{-\lambda^2/2\alpha}}{\sqrt{\alpha\pi}} \int_{\mathbb{R}} e^{-t^2}\, dt = \frac{e^{-\lambda^2/2\alpha}}{\sqrt{\alpha}}
\end{aligned}$$

The next to last step follows from the Cauchy integral formula and the exponential decrease of e^{-z^2} along lines parallel to the x axis.

We now define the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$.

Definition Let $T \in \mathscr{S}'(\mathbb{R}^n)$. Then the Fourier transform of T, denoted by $\hat{T}$, is the tempered distribution defined by $\hat{T}(\varphi) = T(\hat{\varphi})$.

Suppose that h, $\varphi \in \mathscr{S}(\mathbb{R}^n)$, then by the polarization identity and the corollary to Theorem IX.1 we have $(h, \varphi) = (\check{h}, \hat{\varphi})$. Substituting $\check{\bar{g}} = \bar{\check{g}}$ for h, we obtain

$$T_{\hat{g}}(\varphi) = \int \hat{g}(x)\varphi(x)\,dx = \int g(x)\hat{\varphi}(x)\,dx = T_g(\hat{\varphi}) = \hat{T}_g(\varphi)$$

where $T_{\hat{g}}$ and T_g are the distributions corresponding to the functions $\hat{g}$ and g respectively. This shows that the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$ extends the transform we previously defined on $\mathscr{S}(\mathbb{R}^n)$.

Theorem IX.2 The Fourier transform is a one-to-one linear bijection from $\mathscr{S}'(\mathbb{R}^n)$ to $\mathscr{S}'(\mathbb{R}^n)$ which is the unique weakly continuous extension of the Fourier transform on $\mathscr{S}(\mathbb{R}^n)$.

Proof If $\varphi_n \xrightarrow{\mathscr{S}} \varphi$, then by Theorem IX.1, $\hat{\varphi}_n \xrightarrow{\mathscr{S}} \hat{\varphi}$, so $T(\hat{\varphi}_n) \to T(\hat{\varphi})$ for each T in $\mathscr{S}'(\mathbb{R}^n)$. Thus $\hat{T}(\varphi_n) \to \hat{T}(\varphi)$, which shows that $\hat{T}$ is a continuous linear functional on $\mathscr{S}(\mathbb{R}^n)$. Furthermore, if $T_n \xrightarrow{w} T$, then $\hat{T}_n \xrightarrow{w} \hat{T}$ because $T_n(\hat{\varphi}) \to T(\hat{\varphi})$ implies $\hat{T}_n(\varphi) \to \hat{T}(\varphi)$. Thus $T \mapsto \hat{T}$ is weakly continuous.

The remaining properties of $\hat{}$ follow immediately from the corresponding statements on $\mathscr{S}(\mathbb{R}^n)$ (see Problem 19 in Chapter V). ∎

Example 2 We compute the Fourier transform of the derivative of the delta function at $b \in \mathbb{R}$:

$$\begin{aligned}
\hat{\delta}_b'(\varphi) &= \delta_b'(\hat{\varphi}) \\
&= \delta_b\left(-\frac{d}{d\lambda}\hat{\varphi}(\lambda)\right) \\
&= \delta_b\left(\frac{-1}{(2\pi)^{1/2}}\int e^{-i\lambda x}(-ix)\varphi(x)\,dx\right) \\
&= \int\left(\frac{ixe^{-ibx}}{\sqrt{2\pi}}\right)\varphi(x)\,dx
\end{aligned}$$

So, the Fourier transform of δ_b' is the function $ixe^{-ibx}/\sqrt{2\pi}$.

* * *

We now introduce a new operation on functions.

Definitions Suppose that $f, g \in \mathscr{S}(\mathbb{R}^n)$. Then the **convolution** of f and g, denoted by $f * g$, is the function

$$(f * g)(y) = \int_{\mathbb{R}^n} f(y - x)g(x)\,dx$$

The convolution arises in many circumstances (we have already used it in discussing closed operators in Section VIII.1). In Section 4 we use interpolation theorems to prove L^p estimates on the convolution $f * g$ in terms of f and g. In this section we concentrate on the properties of the convolution as a map from $\mathscr{S}(\mathbb{R}^n) \times \mathscr{S}(\mathbb{R}^n)$ to $\mathscr{S}(\mathbb{R}^n)$. Using these properties we show that the convolution can be extended to a map from $\mathscr{S}'(\mathbb{R}^n) \times \mathscr{S}(\mathbb{R}^n)$ to O_M^n, the polynomially bounded C^∞ functions. Convolutions frequently occur when one uses the Fourier transform because the Fourier transform takes products into convolutions (Theorem IX.3b and Theorem IX.4c).

Theorem IX.3

(a) For each $f \in \mathscr{S}(\mathbb{R}^n)$, $g \to f * g$ is a continuous map of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$.

(b) $\widehat{fg} = (2\pi)^{-n/2}\hat{f} * \hat{g}$ and $\widehat{f * g} = (2\pi)^{n/2}\hat{f}\hat{g}$.

(c) For f, g, h, in $\mathscr{S}(\mathbb{R}^n)$, $f * g = g * f$ and $f * (g * h) = (f * g) * h$.

Proof From the polarization identity and the corollary to Theorem IX.1 we find that $(\varphi, \psi) = (\hat{\varphi}, \hat{\psi})$ for $\varphi, \psi \in \mathscr{S}(\mathbb{R}^n)$. Letting $y \in \mathbb{R}^n$ be fixed, we apply this identity to $e^{iy \cdot x}f(x)$ and g obtaining $(e^{iy \cdot x}f, g) = (\widehat{e^{iy \cdot x}f}, \hat{g})$. But

$$(e^{iy \cdot x}f, g) = \int_{\mathbb{R}^n} e^{-iy \cdot x}f(x)g(x)\,dx$$

and

$$(\widehat{e^{iy \cdot x}f}, \hat{g}) = \int_{\mathbb{R}^n} \left(\overline{(2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i\lambda \cdot x + iy \cdot x} \overline{f(x)}\,dx} \right) \hat{g}(\lambda)\,d\lambda$$

$$= \int_{\mathbb{R}^n} \hat{f}(y - \lambda)\hat{g}(\lambda)\,d\lambda$$

which proves that $\widehat{fg} = (2\pi)^{-n/2}\hat{f} * \hat{g}$. Using the inverse Fourier transform this formula may be stated as

$$(2\pi)^{n/2}\widehat{\hat{f}\hat{g}} = f * g$$

This shows that convolution is the composition of the inverse Fourier transform, multiplication by $(2\pi)^{n/2}\check{f}$, and the Fourier transform. It follows that convolution is continuous.

The statements in (c) follow trivially from (b). ∎

In order to extend the map $C_f : g \to f * g$ to $\mathcal{S}'$, we look for a continuous map $\tilde{C}_f : \mathcal{S} \to \mathcal{S}$ so that $\tilde{C}_f' \restriction \mathcal{S} = C_f$. We then define $\tilde{C}_f'$ to be convolution on $\mathcal{S}'$.

Definition Suppose that $f \in \mathcal{S}(\mathbb{R}^n)$, $T \in \mathcal{S}'(\mathbb{R}^n)$ and let $\check{f}(x)$ denote the function, $f(-x)$. Then, the **convolution** of T and f, denoted $T * f$, is the distribution in $\mathcal{S}'(\mathbb{R}^n)$ given by

$$(T * f)(\varphi) = T(\check{f} * \varphi)$$

for all $\varphi \in \mathcal{S}(\mathbb{R}^n)$.

The fact that $g \to \check{f} * g$ is a continuous transformation guarantees that $T * f \in \mathcal{S}'(\mathbb{R}^n)$. The following theorem summarizes the properties of this extended convolution.

Let f_y denote the function $f_y(x) = f(x - y)$ and $\check{f}_y$ the function $f(y - x)$. When f is given by a large expression $(\cdots)$, we will sometimes write $(\cdots)^{\check{}}$ rather than $(\cdot\check{}\cdot)$.

Theorem IX.4 For each $f \in \mathcal{S}(\mathbb{R}^n)$ the map $T \to T * f$ is a weakly continuous map of $\mathcal{S}'(\mathbb{R}^n)$ into $\mathcal{S}'(\mathbb{R}^n)$ which extends the convolution on $\mathcal{S}(\mathbb{R}^n)$. Furthermore,

(a) $T * f$ is a polynomially bounded C^∞ function, i.e. $T * f \in \mathcal{O}_M^n$. In fact, $(T * f)(y) = T(\check{f}_y)$ and

$$D^\beta(T * f) = (D^\beta T) * f = T * D^\beta f \qquad \text{(IX.3)}$$

(b) $(T * f) * g = T * (f * g)$

(c) $\widehat{T * f} = (2\pi)^{n/2}\hat{f}\hat{T}$

Proof Since $T \to T * f$ is defined as the adjoint of a bounded map from $\mathcal{S}$ to $\mathcal{S}$, it is automatically weakly continuous. The fact that it extends the convolution on $\mathcal{S}$ is just a change of variables. The statements (IX.3), (b), and (c), all follow immediately from the corresponding statements for $T \in \mathcal{S}$ and the facts that $\mathcal{S}$ is weakly dense in $\mathcal{S}'$ and that $\mathcal{F}$, D^β, multiplication by $\hat{f}$, and convolution are all weakly continuous on $\mathcal{S}'$.

It remains to prove the first part of (a). Since $T \in \mathscr{S}'(\mathbb{R}^n)$, it follows from the regularity theorem (Theorem V.10) that there is a bounded continuous function h, a positive integer r, and a multi-index β so that

$$T(\check{f}_y) = \int_{\mathbb{R}^n} h(x)(1 + x^2)^r (D^\beta f)(y - x)\, dx$$

Since $D^\beta f \in \mathscr{S}$, $T(\check{f}_y)$ is an infinitely differentiable function of y. The change of variables $\tau = y - x$ shows that

$$\begin{aligned} |T(\check{f}_y)| &\le \|h\|_\infty \int_{\mathbb{R}^n} (1 + x^2)^r |(D^\beta f)(y - x)|\, dx \\ &= \|h\|_\infty \int_{\mathbb{R}^n} (1 + (y - \tau)^2)^r |D^\beta f(\tau)|\, d\tau \end{aligned}$$

from which it follows easily that $y \mapsto T(\check{f}_y)$ is polynomially bounded. A similar proof works for the derivatives of $y \mapsto T(\check{f}_y)$. Thus $T(\check{f}_y) \in O_M^n$.

Suppose that a distribution $S \in \mathscr{S}'(\mathbb{R}^n)$ is given by a polynomially bounded continuous function s. Then, using Fubini's theorem we find that for $\varphi \in \mathscr{S}(\mathbb{R}^n)$

$$\begin{aligned} (S * f)(\varphi) &\equiv S(\check{f} * \varphi) \\ &= \int s(x) \left(\int \check{f}(x - y)\varphi(y)\, dy \right) dx \\ &= \int \left(\int s(x)\check{f}_y(x)\, dx \right) \varphi(y)\, dy \\ &= (S(\check{f}_y))(\varphi) \end{aligned}$$

so $S * f = S(\check{f}_y)$. By the regularity theorem $T = D^\alpha S$ for some such S. Thus by (IX.3)

$$\begin{aligned} T * f = (D^\alpha S) * f &= S * D^\alpha f \\ &= S((D^\alpha f)^\vee_y) \\ &= (-1)^{|\alpha|} S(D^\alpha(\check{f}_y)) \\ &= D^\alpha S(\check{f}_y) \\ &= T(\check{f}_y) \end{aligned}$$

This completes the proof. ∎

Theorem IX.5 Let $T \in \mathscr{S}'(\mathbb{R}^n)$ and $f \in \mathscr{S}(\mathbb{R}^n)$. Then $\widehat{fT} \in O_M^n$ and $\widehat{fT}(k) = (2\pi)^{-n/2} T(f e^{-ik\cdot x})$. In particular, if T has compact support and $\psi \in \mathscr{S}(\mathbb{R}^n)$ is identically one on a neighborhood of the support of T, then

$$\hat{T}(k) = (2\pi)^{-n/2} T(\psi e^{-ik\cdot x})$$

Proof By Theorem IX.4c and the Fourier inversion formula we have $\widehat{fT} = (2\pi)^{-n/2} \hat{f} * \hat{T}$. Thus $\widehat{fT} \in O_M^n$ and

$$\begin{aligned} \widehat{fT}(k) &= (2\pi)^{-n/2} \hat{T}(\check{\hat{f}}_k) \\ &= (2\pi)^{-n/2} T(e^{-ik\cdot x} f) \end{aligned}$$

∎

We remark that one can also define the convolution of a distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ with an $f \in \mathscr{D}(\mathbb{R}^n)$ by $(T * f)(y) = T(\check{f}_y)$. A proof similar to the proof of Theorem IX.4 shows that $T * f$ is a (not necessarily polynomially bounded) C^∞ function and that (IX.3) holds.

We have already introduced the term "approximate identity" in Section VIII.1; we now define it formally.

Definition Let $j(x)$ be a positive C^∞ function whose support lies in the sphere of radius one about the origin in $\mathbb{R}^n$ and which satisfies $\int j(x)\,dx = 1$. The sequence of functions $j_\varepsilon(x) = \varepsilon^{-n} j(x/\varepsilon)$ is called an **approximate identity.**

Proposition Suppose $T \in \mathscr{S}'(\mathbb{R}^n)$ and let $j_\varepsilon(x)$ be an approximate identity. Then $T * j_\varepsilon \to T$ weakly as $\varepsilon \to 0$.

Proof If $\varphi \in \mathscr{S}(\mathbb{R}^n)$, then $(T * j_\varepsilon)(\varphi) = T(\tilde{j}_\varepsilon * \varphi)$, so it is sufficient to show that $\tilde{j}_\varepsilon * \varphi \xrightarrow{\mathscr{S}(\mathbb{R}^n)} \varphi$. To do this it is sufficient to show that $(2\pi)^{n/2} \hat{j}_\varepsilon \hat{\varphi} \rightrightarrows \hat{\varphi}$. Since $\hat{j}_\varepsilon(\lambda) = \hat{j}(\varepsilon\lambda)$ and $\hat{j}(0) = (2\pi)^{-n/2}$, it follows that $(2\pi)^{n/2} \hat{j}_\varepsilon(x)$ converges to 1 uniformly on compact sets and is uniformly bounded. Similarly, $D^\alpha \hat{j}_\varepsilon$ converges uniformly to zero. We conclude that $(2\pi)^{n/2} \hat{j}_\varepsilon \hat{\varphi} \rightrightarrows \hat{\varphi}$. ∎

IX.2 The range of the Fourier transform: Classical spaces

We have defined the Fourier transform on $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{S}'(\mathbb{R}^n)$. In this section, Section IX.3, and Section IX.9, we investigate the range of the Fourier transform when it is restricted to various subsets of $\mathscr{S}'(\mathbb{R}^n)$. These

questions are natural and have historical interest, but more important, characterizing the range of the Fourier transform is very useful. One is often able to obtain information about the Fourier transform of a function and one would like to know what this says about the function itself. We begin with two theorems which follow easily from the work that we have already done in Section IX.1.

Theorem IX.6 (the Plancherel theorem) The Fourier transform extends uniquely to a unitary map of $L^2(\mathbb{R}^n)$ onto $L^2(\mathbb{R}^n)$. The inverse transform extends uniquely to its adjoint.

Proof The corollary to Theorem IX.1 states that if $f \in \mathscr{S}(\mathbb{R}^n)$, then $\|f\|_2 = \|\hat{f}\|_2$. Since $\mathscr{F}[\mathscr{S}] = \mathscr{S}$, $\mathscr{F}$ is a surjective isometry on $L^2(\mathbb{R}^n)$. ∎

Theorem IX.7 (the Riemann–Lebesgue lemma) The Fourier transform extends uniquely to a bounded map from $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$, the continuous functions vanishing at ∞.

Proof For $f \in \mathscr{S}(\mathbb{R}^n)$, we know that $\hat{f} \in \mathscr{S}(\mathbb{R}^n)$ and thus $\hat{f} \in C_\infty(\mathbb{R}^n)$. The estimate

$$\|\hat{f}\|_\infty \leq (2\pi)^{-n/2}\|f\|_1$$

is trivial. The Fourier transform is thus a bounded linear map from a dense set of $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$. By the B.L.T. theorem, $\hat{}$ extends uniquely to a bounded linear transformation of $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$. ∎

We remark that the Fourier transform takes $L^1(\mathbb{R}^n)$ into, but not onto $C_\infty(\mathbb{R}^n)$ (Problem 16).

A simple argument with test functions shows that the extended transform on $L^1(\mathbb{R}^n)$ and $L^2(\mathbb{R}^n)$ is the restriction of the transform on $\mathscr{S}'(\mathbb{R}^n)$, but it is useful to have an explicit integral representation. For $f \in L^1(\mathbb{R}^n)$, this is easy since we can find $f_m \in \mathscr{S}(\mathbb{R}^n)$ so that $\|f - f_m\|_1 \to 0$. Then, for each λ,

$$\begin{aligned}\hat{f}(\lambda) &= \lim_{m\to\infty} (\hat{f}_m(\lambda)) \\ &= \lim_{m\to\infty} \left\{ \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\lambda\cdot x} f_m(x)\, dx \right\} \\ &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\lambda\cdot x} f(x)\, dx\end{aligned}$$

So, the Fourier transform of a function in $L^1(\mathbb{R}^n)$ is given by the usual formula.

Next, suppose $f \in L^2(\mathbb{R}^n)$ and let

$$\chi_R(x) = \begin{cases} 1 & |x| \leq R \\ 0 & |x| > R \end{cases}$$

Then $\chi_R f \in L^1(\mathbb{R}^n)$ and $\chi_R f \xrightarrow[R\to\infty]{L^2} f$, so by the Plancherel theorem $\widehat{\chi_R f} \xrightarrow[R\to\infty]{L^2} \hat{f}$. For $\chi_R f$ we have the usual formula; thus

$$\hat{f}(\lambda) = \operatorname*{l.i.m.}_{R\to\infty} (2\pi)^{-n/2} \int_{|x|\leq R} e^{-i\lambda\cdot x} f(x)\, dx$$

where by "l.i.m." we mean the limit in the L^2-norm. Sometimes we will dispense with $|x| \leq R$ and just write

$$\hat{f}(\lambda) = \operatorname{l.i.m.}(2\pi)^{-n/2} \int e^{-i\lambda\cdot x} f(x)\, dx$$

for functions $f \in L^2(\mathbb{R}^n)$.

We have proven above that $L^2(\mathbb{R}^n) \xrightarrow{\hat{}} L^2(\mathbb{R}^n)$ and $L^1(\mathbb{R}^n) \xrightarrow{\hat{}} L^\infty(\mathbb{R}^n)$ and in both cases $\hat{}$ is a bounded operator. It is exactly in situations like this that one can use the interpolation theorems which we will prove in the Appendix to Section 4.

Theorem IX.8 (Hausdorff-Young inequality) Suppose $1 \leq q \leq 2$, and $p^{-1} + q^{-1} = 1$. Then the Fourier transform is a bounded map of $L^q(\mathbb{R}^n)$ to $L^p(\mathbb{R}^n)$ and its norm is less than or equal to $(2\pi)^{n(1/2-1/q)}$.

Proof We use the Riesz–Thorin theorem (Theorem IX.17) with $q_0 = 2 = p_0$, $p_1 = \infty$, and $q_1 = 1$. Since $\|\hat{f}\|_2 = \|f\|_2$ and $\|\hat{f}\|_\infty \leq (2\pi)^{-n/2}\|f\|_1$, we conclude that $\|\hat{f}\|_{p_t} \leq C_t \|f\|_{q_t}$ where $p_t^{-1} = (1-t)/2$, $q_t^{-1} = (1-t)/2 + t = 1 - p_t^{-1}$, and $\log C_t = t \log(2\pi)^{-n/2}$. ∎

* * *

We now come to another natural question. What are the Fourier transforms of the finite positive measures on $\mathbb{R}^n$? Suppose that we define

$$\hat{\mu}(\lambda) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i\lambda\cdot x}\, d\mu(x)$$

Then, if $\varphi \in \mathscr{S}(\mathbb{R}^n)$,

$$\int_{\mathbb{R}^n} \hat{\mu}(\lambda)\varphi(\lambda)\, d\lambda = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} e^{-i\lambda \cdot x}\, d\mu(x) \right) \varphi(\lambda)\, d\lambda$$

$$= (2\pi)^{-n/2} \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} e^{-i\lambda \cdot x} \varphi(\lambda)\, d\lambda \right) d\mu(x)$$

$$= \int_{\mathbb{R}^n} \hat{\varphi}(x)\, d\mu(x)$$

so this definition coincides with the restriction of the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$ to the positive measures. Suppose $\lambda_1, \ldots, \lambda_N \in \mathbb{R}^n$ and $\xi = \langle \xi_1, \xi_2, \ldots, \xi_N \rangle \in \mathbb{C}^N$. Then

$$\sum_{i,j=1}^{N} \hat{\mu}(\lambda_i - \lambda_j)\xi_j \xi_i = \int \left| \sum_{i=1}^{N} \xi_i e^{-i\lambda_i \cdot x} \right|^2 d\mu(x) \geq 0$$

This shows that the function $\hat{\mu}(\lambda)$ has the property that for any $\lambda_1, \ldots, \lambda_N \in \mathbb{R}^n$, $\{\hat{\mu}(\lambda_i - \lambda_j)\}$ is the matrix of a positive operator on $\mathbb{C}^N$. Furthermore, by the dominated convergence theorem, $\hat{\mu}$ is continuous, and since

$$|\hat{\mu}(\lambda)| \leq (2\pi)^{-n/2} \int_{\mathbb{R}^n} |e^{-i\lambda \cdot x}|\, d\mu(x)$$

$$= (2\pi)^{-n/2} \mu(\mathbb{R}^n)$$

$\hat{\mu}(\cdot)$ is also bounded.

Definition A complex-valued, bounded, continuous function f on $\mathbb{R}^n$ that has the property that $\{f(\lambda_i - \lambda_j)\}_{i,j}$ is a positive matrix on $\mathbb{C}^N$ for each N and all $\lambda_1, \ldots, \lambda_N \in \mathbb{R}^n$ is called a **function of positive type.**

There are three properties of functions of positive type which follow easily from the definition. Letting $N = 1$, $x \in \mathbb{R}^N$,

$$(1) \quad f(0) \geq 0$$

since $f(0)$ is a positive operator on $\mathbb{C}^1$. Letting $N = 2$, and choosing $\lambda_1 = x$, $\lambda_2 = 0$, we see that the matrix

$$\begin{pmatrix} f(0) & f(x) \\ f(-x) & f(0) \end{pmatrix}$$

must be positive and therefore self-adjoint with positive determinant. This implies that

$$(2) \quad f(x) = \overline{f(-x)}$$
$$(3) \quad |f(x)| \leq f(0)$$

Notice that in proving these three properties we did not use the fact that $f(x)$ is bounded, so we could have left out the word *bounded* in the definition and recovered boundedness from (3) above. It is clear that any convex combinations or scalar multiples of functions of positive type again give functions of positive type, so these functions form a cone.

Theorem IX.9 (Bochner's theorem) The set of Fourier transforms of the finite, positive measures on $\mathbb{R}^n$ is exactly the cone of functions of positive type.

Proof We do not give Bochner's original proof but rather an easy, interesting argument based on Stone's theorem. We have already shown that the Fourier transforms of finite positive measures are functions of positive type. We need to prove the converse. Suppose f is of positive type. Let $\mathscr{K}$ denote the set of complex-valued functions on $\mathbb{R}^n$ which vanish except at a finite number of points. Then

$$(\psi, \varphi)_f = \sum_{x, y \in \mathbb{R}^n} f(x - y)\overline{\psi(x)}\varphi(y)$$

has all the properties of a well-defined inner product except that we may have $(\varphi, \varphi)_f = 0$ for some $\varphi \neq 0$. If we let $\mathscr{N}$ be the set of such φ, then $\mathscr{K}/\mathscr{N}$ is a well-defined pre-Hilbert space under $(\cdot, \cdot)_f$. Suppose that $t \in \mathbb{R}^n$ and define U_t on $\mathscr{K}$ by $(U_t\varphi)(x) = \varphi(x - t)$. Since U_t preserves the form $(\cdot, \cdot)_f$, it takes equivalence classes into equivalence classes and thus restricts to an isometry on $\mathscr{K}/\mathscr{N}$. Since the same is true of U_{-t}, this isometry has dense range and thus extends to a unitary operator $\tilde{U}_t$ on $\mathscr{H} = \overline{\mathscr{K}/\mathscr{N}}$. Furthermore, $\tilde{U}_{t+s} = \tilde{U}_t\tilde{U}_s$, $\tilde{U}_0 = I$, and because of the continuity of f, $\tilde{U}_t$ is strongly continuous. Thus the map $t \to \tilde{U}_t$ satisfies the hypotheses of Theorem VIII.12 (the generalization of Stone's theorem). Therefore, there is a projection-valued measure P_λ, on $\mathbb{R}^n$ so that

$$(\varphi, \tilde{U}_t\psi)_f = \int_{\mathbb{R}^n} e^{it\cdot\lambda}\, d(\varphi, P_\lambda\psi)_f$$

Let $\tilde{\varphi}_0$ denote the equivalence class containing the function

$$\varphi_0(x) = \begin{cases} 1, & x = 0 \\ 0, & x \neq 0 \end{cases}$$

Then

$$f(t) = (\tilde{U}_t\tilde{\varphi}_0, \tilde{\varphi}_0)_f = (\tilde{\varphi}_0, \tilde{U}_{-t}\tilde{\varphi}_0)_f = \int e^{-it\cdot\lambda}\, d(\tilde{\varphi}_0, P_\lambda\tilde{\varphi}_0)_f$$

so we have displayed f as the Fourier transform of a finite positive measure. ∎

The notion of positive type may be generalized to distributions. If $f(x)$ is a bounded continuous function, then $f(x)$ will be of positive type if and only if

$$\int\int f(x-y)\overline{\varphi(y)}\varphi(x)\,dx\,dy \geq 0 \tag{IX.4}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^n)$. To see this one need only approximate the integral in (IX.4) by a Riemann sum. This condition can be rewritten as

$$\iint f(\tau)\overline{\varphi(x-\tau)}\varphi(x)\,d\tau\,dx = \int f(\tau)(\tilde{\bar{\varphi}} * \varphi)(\tau)\,d\tau \geq 0 \tag{IX.5}$$

where $\tilde{\varphi}$ is the function $\tilde{\varphi}(x) = \varphi(-x)$. This suggests the following definition.

Definition A distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ is said to be of **positive type** if $T(\tilde{\bar{\varphi}} * \varphi) \geq 0$ for all $\varphi \in \mathscr{D}(\mathbb{R}^n)$.

The following generalization of Bochner's theorem is due to Schwartz. This theorem is particularly interesting since it implies that certain ordinary distributions must be tempered. The proof is sketched in Problem 20 (or see the Notes for a reference).

Theorem IX.10 (the Bochner–Schwartz theorem) A distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ is a distribution of positive type if and only if $T \in \mathscr{S}'(\mathbb{R}^n)$ and T is the Fourier transform of a positive measure of at most polynomial growth.

If $f(x)$ is a function of positive type, then this theorem implies that the weak derivatives $(-\Delta)^m f$ are all distributions of positive type. For $\hat{f} = \mu$, a finite measure by Theorem IX.9, and $\widehat{(-\Delta)^m f} = |x|^{2m}\mu$, a positive measure of polynomial growth.

Finally, we determine which bounded measurable functions are distributions of positive type. A bounded measurable function f on $\mathbb{R}^n$ is said to be of **weak positive type** if (IX.4) holds. Since (IX.5) follows from (IX.4), the distribution

$$T_f(\varphi) = \int f(x)\varphi(x)\,dx$$

is of positive type and therefore $\hat{T}_f = \mu$, a polynomially bounded positive

measure. If $j_\varepsilon(x)$ is an approximate identity that is symmetric about the origin, then

$$\begin{aligned}\|f\|_\infty \geq T_f(j_\varepsilon * j_\varepsilon) &= \hat{T}_f(\widetilde{(j_\varepsilon * j_\varepsilon)}) \\ &= (2\pi)^{n/2}\mu(|\check{j}_\varepsilon(x)|^2) \\ &= (2\pi)^{n/2}\int |\check{j}_\varepsilon(x)|^2\, d\mu(x)\end{aligned}$$

On each compact subset of $\mathbb{R}^n$, $\check{j}_\varepsilon(x)$ converges uniformly to $(2\pi)^{-n/2}$ as $\varepsilon \to 0$, so the μ-measure of any compact set is less than $(2\pi)^{n/2}\|f\|_\infty$, so μ is finite.

We now come to the interesting point. Since μ is finite, its Fourier transform is a continuous function of positive type. Since μ and f must coincide a.e., we have proven:

Proposition A bounded function of weak positive type is equal almost everywhere to a continuous function of positive type.

IX.3 The range of the Fourier transform: Analyticity

In this section we investigate the connection between the decay properties of a function or distribution at infinity and the analyticity properties of its Fourier transform. The most extreme form of decay at infinity is to have compact support. We will prove the Paley–Wiener and Schwartz theorems which characterize explicitly the Fourier transforms of C^∞ functions and distributions with compact support. We then state two theorems relating exponential decay to analyticity properties of the Fourier transform. We close the section by characterizing the Fourier transforms of tempered distributions whose supports lie in symmetric cones. There are many other theorems of this genre; some of them are discussed in the Notes.

Suppose that $f \in C_0^\infty(\mathbb{R}^n)$. Then for all $\zeta = \langle \zeta_1, \ldots, \zeta_n \rangle \in \mathbb{C}^n$, the integral

$$\hat{f}(\zeta) = (2\pi)^{-n/2}\int e^{-i\zeta\cdot x} f(x)\, dx$$

is well defined. Furthermore, $\hat{f}(\zeta)$ is an entire analytic function of the n complex variables $\zeta_1, \zeta_2, \ldots, \zeta_n$ since we can differentiate under the

integral sign. In addition, if the support of f is contained in the sphere of radius R, then an integration by parts yields

$$\prod_{i=1}^{n}(i\zeta_i)^{\alpha_i}\hat{f}(\zeta) = (2\pi)^{-n/2}\int_{|x|\le R} e^{-i\zeta\cdot x}D^{\alpha}f(x)\,dx$$

Taking the absolute value of both sides and using the fact that $\hat{f}(\zeta)$ is bounded on the set $\{\zeta \mid |\operatorname{Im}\zeta| < \varepsilon\}$, we easily conclude that for each N,

$$|\hat{f}(\zeta)| \le \frac{C_N e^{R|\operatorname{Im}\zeta|}}{(1+|\zeta|)^N} \qquad \text{for all } \zeta \in \mathbb{C}^n$$

where C_N is a constant that depends on N and f. The interesting fact is that these estimates are not only necessary but also sufficient for f to be in $C_0^\infty(\mathbb{R}^n)$.

Theorem IX.11 (the Paley–Wiener theorem) An entire analytic function of n complex variables $g(\zeta)$ is the Fourier transform of a $C_0^\infty(\mathbb{R}^n)$ function with support in the ball $\{x \mid |x| \le R\}$ if and only if for each N there is a C_N so that

$$|g(\zeta)| \le \frac{C_N e^{R|\operatorname{Im}\zeta|}}{(1+|\zeta|)^N} \tag{IX.6}$$

for all $\zeta \in \mathbb{C}^n$.

Proof We have already proven the "only if" part. Suppose that g is entire and satisfies estimates of the form (IX.6). Let $\zeta = \lambda + i\eta$, where $\lambda, \eta \in \mathbb{R}^n$. Then for each η, $g(\lambda + i\eta)$ is in $\mathscr{S}(\mathbb{R}^n)$ as a function of λ, since the derivatives fall off polynomially by (IX.6) and the Cauchy formula. Let

$$f(x) = (2\pi)^{-n/2}\int_{\mathbb{R}^n} e^{ix\cdot\lambda}g(\lambda)\,d\lambda \tag{IX.7}$$

Then by Theorem IX.1, $f \in \mathscr{S}(\mathbb{R}^n)$ and $g(\lambda) = \hat{f}(\lambda)$. We want to show that $f(x)$ has support in the ball of radius R. Because of the estimates (IX.6) and Cauchy's theorem, we can shift the region of integration in (IX.7) so that

$$f(x) = (2\pi)^{-n/2}\int_{\mathbb{R}^n} e^{i(\lambda+i\eta)\cdot x}g(\lambda+i\eta)\,d\lambda \tag{IX.8}$$

Thus, by (IX.6)

$$|f(x)| \le e^{R|\eta|-x\cdot\eta}(2\pi)^{-n/2}\int \frac{C_N}{(1+|\lambda+i\eta|)^N}\,d\lambda$$

$$\le e^{R|\eta|-x\cdot\eta}(2\pi)^{-n/2}\int \frac{C_N}{(1+|\lambda|)^N}\,d\lambda$$

where we have chosen N large enough so that the integral on the right is finite. Now, $f(x)$ does not depend on η, so if we let $\eta \to \infty$ in an appropriate direction, we conclude that $|f(x)| = 0$ if $|x| > R$. ∎

This theorem has a natural generalization to the distributions with compact support. Recall that a distribution $T \in \mathscr{S}'(\mathbb{R}^n)$ has support in a closed set K if and only if $T(\varphi) = 0$ for every test function φ with support in $\mathbb{R}^n \backslash K$. If K is compact, then T is said to have **compact support**. The set of distributions with compact support is the dual space of $\mathscr{E}(\mathbb{R}^n)$ (see Problems 39 and 40 of Chapter V).

Theorem IX.12 A distribution $T \in \mathscr{S}'(\mathbb{R}^n)$ has compact support if and only if $\hat{T}$ has an analytic continuation to an entire analytic function of n variables $\hat{T}(\zeta)$ that satisfies

$$|\hat{T}(\zeta)| \leq C(1 + |\zeta|)^N e^{R|\operatorname{Im}\zeta|} \tag{IX.9}$$

for all $\zeta \in \mathbb{C}^n$ and some constants C, N, R. Moreover, if (IX.9) holds, the support of T is contained in the ball of radius R.

Proof Suppose that $T \in \mathscr{S}'(\mathbb{R}^n)$ has compact support and let φ be a $C_0^\infty(\mathbb{R}^n)$ function which is equal to one on the support of T. Define $F(\zeta) = T[(2\pi)^{-n/2} e^{-i\zeta \cdot x}\varphi(x)]$. By Theorem IX.5, $F(\lambda + i0)$ is the Fourier transform of T. Furthermore, since

$$\left(\frac{\exp(-i(x_j(\zeta_j + h_j) + \sum_{k \neq j} \zeta_k x_k))\varphi(x) - e^{-i\zeta \cdot x}\varphi(x)}{h_j}\right)$$

$$\xrightarrow{\mathscr{S}(\mathbb{R}^n)} -ix_j e^{-i\zeta \cdot x}\varphi(x)$$

and $T \in \mathscr{S}'(\mathbb{R}^n)$, $F(\zeta)$ is differentiable in the complex sense in each variable and is thus entire.

Since $T \in \mathscr{S}'(\mathbb{R}^n)$,

$$|T(f)| \leq C_1 \sum_{\substack{|\alpha| \leq N \\ |\beta| \leq N}} \|x^\alpha D^\beta f\|_\infty$$

for some N and C_1 and all $f \in \mathscr{S}(\mathbb{R}^n)$. Thus, if φ has support in the sphere of radius R, then

$$|F(\zeta)| \leq C_2(1 + R^n)(1 + |\zeta|^N)e^{|\operatorname{Im}\zeta|R}$$

Conversely, suppose that $F(\zeta)$ is an entire function satisfying the estimate (IX.9). Then $F(\lambda + i0) \in \mathscr{S}'(\mathbb{R}^n)$, so it is the Fourier transform of some $T \in \mathscr{S}'(\mathbb{R}^n)$. Let $j_\varepsilon(x)$ be an approximate identity. Then by Theorem IX.4,

$\widehat{T * j_\varepsilon} = (2\pi)^{-n/2}\hat{j}_\varepsilon(\lambda)F(\lambda)$. Since j_ε has compact support in $\{x \mid |x| \leq \varepsilon\}$, we know by the Paley-Wiener theorem, that for each M we can find a constant C_M so that

$$|\hat{j}_\varepsilon(\zeta)| \leq \frac{C_M}{(1 + |\zeta|)^{N+M}} e^{\varepsilon|\operatorname{Im}\zeta|}$$

Therefore

$$|(2\pi)^{-n/2}\hat{j}_\varepsilon(\zeta)F(\zeta)| \leq \frac{C_M\, Ce^{(R+\varepsilon)|\operatorname{Im}\zeta|}}{(1 + |\zeta|)^N}$$

which implies (again by the Paley-Wiener theorem) that the support of $T * j_\varepsilon$ is contained in the sphere of radius $R + \varepsilon$. Since ε is arbitrary and $(T * j_\varepsilon) \to T$ weakly, we conclude that the support of T is contained in the sphere of radius R about the origin. ∎

One natural way to extend the above theorems is to replace "compact support" with some weaker notion of decay at infinity. The following pair of theorems (whose proofs are outlined in Problem 76) will be used in Chapter XIII to prove the exponential decay of bound states of atomic Hamiltonians.

Theorem IX.13 Let f be in $L^2(\mathbb{R}^n)$. Then $e^{b|x|}f \in L^2(\mathbb{R}^n)$ for all $b < a$ if and only if $\hat{f}$ has an analytic continuation to the set $\{\zeta \mid |\operatorname{Im}\zeta| < a\}$ with the property that for each $\eta \in \mathbb{R}^n$ with $|\eta| < a$, $\hat{f}(\cdot + i\eta) \in L^2(\mathbb{R}^n)$ and for any $b < a$

$$\sup_{|\eta| \leq b} \|\hat{f}(\cdot + i\eta)\|_2 < \infty$$

Theorem IX.14 Let T be in $\mathscr{S}'(\mathbb{R}^n)$. Suppose that $\hat{T}$ is a function with an analytic continuation to the set $\{\zeta \mid |\operatorname{Im}\zeta| < a\}$ for some $a > 0$. Suppose further that for each $\eta \in \mathbb{R}^n$ with $|\eta| < a$, $\hat{T}(\cdot + i\eta) \in L^1(\mathbb{R}^n)$ and for any $b < a$, $\sup_{|\eta| < b} \|\hat{T}(\cdot + i\eta)\|_1 < \infty$. Then T is a bounded continuous function and for any $b < a$, there is a constant C_b so that

$$|T(x)| \leq C_b e^{-b|x|}$$

Paley-Wiener theorems are useful for understanding certain kinds of analytic completion theorems in the theory of several complex variables. The basic phenomenon is illustrated in the following simple example: Let D_r be the

Theorem IX.14.2 (degenerate tube theorem) Let $T_1(x_1, z_2)$ and $T_2(z_1, x_2)$ be tempered distributions in the x variables ($x \in \mathbb{R}^n$) and polynomially bounded analytic functions in the z variables in $\{z \in \mathbb{C}^n | |\operatorname{Im} z| < 1\}$, i.e., for each z_2, $T_1(x_1, z_2)$ is a distribution in x_1 and $\int g(x_1)T(x_1, z_2)\,dx_1$ is analytic. Suppose that $T_1(x_1, x_2 + i0) = T_2(x_1 + i0, x_2)$ as distributions in the two variables. Then there exists a function $f(z_1, z_2)$ analytic in $\mathcal{T}(\tilde{S})$ with $\tilde{S} = \{\langle y_1, y_2\rangle | |y_1| + |y_2| < 1\}$ so that

$$T_1(x_1, z_2) = f(x_1 + i0, z_2) \qquad \text{and} \qquad T_2(z_1, x_2) = f(z_1, x_2 + i0)$$

Proof Let $g(\lambda) = \check{T}_1(\cdot, \cdot + i0)$. Then, by hypothesis, $e^{\theta\lambda_1}g(\lambda)$ and $e^{\theta\lambda_2}g(\lambda)$ are in $\mathcal{S}'$ for $-1 < \theta < 1$ so $e^{a\cdot\lambda}g(\lambda) \in \mathcal{S}'$ for $|a_1| + |a_2| < 1$, proving the result. ∎

NOTES

Section IX.1 J. Fourier's original argument for the inversion formula appears in his classic *La Théorie Analytique de Chaleur*, Didot, Paris, 1822. Although his argument would not be considered a "rigorous proof" by modern standards, it contained the main ideas of the proof we have presented. The approach of first defining the Fourier transform on $\mathcal{S}(\mathbb{R}^n)$ and $\mathcal{S}'(\mathbb{R}^n)$ and then restricting to the classical L^p spaces is due to L. Schwartz and is described in *Théorie des Distributions*, Vol. II, Hermann, Paris, 1954. Schwartz's lucid book is the basic reference for the study of the Fourier transform on spaces of distributions and the theory of convolutions of distributions.

The Hermite expansion discussed in the Appendix to Section V.3 can be used to provide short proofs of the Fourier inversion and Plancherel theorems since $\hat{\varphi}_n(k) = (-i)^n\varphi_n(k)$.

Section IX.2 The Riemann–Lebesgue lemma was first proven for a restricted class of functions in B. Riemann, "Ueber der Darstellbarkeit einer Function durch einen trigonometrische Reihe" in *Math. Werke*, Teubner, 1876, pp. 213–253, and for all of L^1 in H. Lebesgue, "Sur les Séries Trigonométriques," *Ann. Sci. Ecole Norm. Sup.* 20 (1903), 453–485. The Plancherel theorem appears in M. Plancherel, "Contribution à l'étude de la représentation d'un fonction arbitraire par des intégrales définies," *Rend. Circ. Mat. Palermo* 30 (1910), 289–335. The Hausdorff–Young theorem was first proven in W. Young: "Sur la généralisation du théorème de Parseval," *C. R. Acad. Sci. Paris Sér. A-B* 155 (1912), 30–33; and extended in F. Hausdorff, "Eine Ausdehnung des Parselvalschen Satzes über Fourierreihen," *Math. Z.* 16 (1923), 163–169.

The original proof of Bochner's theorem appears in S. Bochner, *Vorlesungen über Fouriersche Integrale*, Akademie-Verlag, Berlin, 1932. For a proof of the generalization to distributions, see Schwartz's book. The proof of Bochner's theorem which we give depends on Stone's theorem. Conversely, it is possible to derive Stone's theorem from Bochner's theorem, see E. Hopf: *Ergodentheorie*, Springer-Verlag, Berlin, 1937, or F. Riesz and B. Sz.-Nagy: *Functional Analysis*, Ungar, New York, 1955.

In some sense, the "natural" setting for the L^p theory of the Fourier transform is on an arbitrary locally compact abelian group; see Chapters XIV and XV.

Section IX.3 The close relationship between the support properties of a function and the analyticity properties of its Fourier transform was first developed by R. Paley and N. Wiener in *Fourier Transforms in the Complex Domain*, Amer. Math. Soc. Colloqium Publication, Providence, Rhode Island, 1934. Their work concerned L^2 functions and L^2 boundary values (see below). Nevertheless, a whole class of theorems relating support properties to analyticity properties are usually called Paley-Wiener theorems. The connection between analyticity and the Fourier Transform was further studied by E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals*, Oxford Univ. Press (Clarendon), London and New York, 1937. The generalization to distributions with compact support was first proven in L. Schwartz, "Transformation de Laplace des distributions," *Comm. Sém. Math. Lund*, tome suppl. dédié à M. Riesz (1952). A more detailed relation between support and analyticity for functions supported on compact, convex, balanced sets is given in Problem 22.

For additional discussion of the phenemona of analytic completion, see: S. Bochner and W. T. Martin, *Several Complex Variables*, Princeton Univ. Press, Princeton, New Jersey, 1948; R. Gunning and H. Rossi, *Analytic Functions of Several Complex Variables*, Prentice-Hall, Englewood Cliffs, New Jersey, 1965; L. Nachbin, *Holomorphic Functions, Domains of Holomorphy and Local Properties*, North Holland, Amsterdam, 1970; L. Hörmander, *An Introduction to Complex Analysis in Several Variables*, Van Nostrand, Princeton, New Jersey, 1966. For applications to quantum field theory, see the Epstein article and Wightman's *J. Indian Math. Soc.* article quoted in the Notes to Section IX.8.

Bochner's tube theorem is due to S. Bochner, "A Theorem on Analytic Continuation of Functions in Several Variables," *Ann. Math.* **39** (1938), 14–19. The connection between tube theorems and the Paley-Wiener theorem has been noted by E. Stein and collaborators; see E. M. Stein and G. Weiss, *Introduction to Fourier Analysis on Euclidean Spaces*, Princeton Univ. Press, Princeton, New Jersey, 1971. In particular, the degenerate tube theorem was proven using these ideas by R. A. Kunze and E. M. Stein in "Uniformly Bounded Representations, II," *Amer. J. Math.* **83** (1961), 723–786 (see Lemma 21). Independently, Malgrange and Zerner proved this result using more classical methods; see H. Epstein's article.

PROBLEMS

1. Find the Fourier transform of $3x^2 + 1$.

†2. Give the details of the convergence of the Riemann sum to the integral at the end of the proof of Theorem IX.1.

3. (a) Let R be a rotation and R^t its transpose. Let $f \in \mathscr{S}$. Prove that $\widehat{f \circ R} = \hat{f} \circ R^t$.
   (b) Let D_λ be the map $D_\lambda x = \lambda x$ on $\mathbb{R}^n$. Let $f \in \mathscr{S}(\mathbb{R}^n)$. Prove that

$$\widehat{f \circ D_\lambda} = \lambda^{-n} \hat{f} \circ D_{\lambda^{-1}}$$

   (c) Let $T \in \mathscr{S}'(\mathbb{R}^n)$. Prove that

$$\widehat{(T \circ R)} = \hat{T} \circ R^t, \qquad \widehat{T \circ D_\lambda} = \lambda^{-n} \hat{T} \circ D_{\lambda^{-1}}$$

4. Compute the Fourier transform of $\mathscr{P}(1/x)$, the Cauchy principle part, by using Equation (V.4).

5. Compute the Fourier transform of $f(x) = e^{-\alpha x^2/2}$ as follows:
   (a) Prove that $-\lambda \hat{f}(\lambda) = \alpha \, d\hat{f}(\lambda)/d\lambda$ and conclude that $\hat{f}(\lambda) = ce^{-\lambda^2/2\alpha}$

polydisk $\{\langle z, w\rangle \mid |z| < r, |w| < r\}$ in $\mathbb{C}^2$. Suppose that f is an analytic function of two variables in the "polyannulus" $D_1 \backslash \bar{D}_{\frac{1}{2}}$. Then for each z with $\frac{1}{2} < |z| < 1$, $g_z(w) \equiv f(z, w)$ is analytic in the unit disk and for each z with $|z| \leq \frac{1}{2}$, $g_z(w)$ is analytic in the annulus $\frac{1}{2} < w < 1$. Thus for each z there is a Laurant expansion

$$g_z(w) = \sum_{n=-\infty}^{\infty} a_n(z) w^n$$

with $a_n(z) = 0$ for $n < 0$ and $1 > |z| > \frac{1}{2}$. But the $a_n(z)$ are easily seen to be analytic functions of z so that $a_n(z) = 0$ for $n < 0$ and $|z| < 1$. It follows that f has a continuation from $D_1 \backslash \bar{D}_{\frac{1}{2}}$ to all of D_1! This is in striking contrast to the case of one variable where given any open connected set $\Omega \subset \mathbb{C}$, one can find an f that is analytic on Ω and on no larger set.

Definition An open connected set $\Omega \subset \mathbb{C}^n$ is called a **holomorphy domain** if and only if for any $w \notin \Omega$, there exists a function f analytic in Ω with no continuation to w. Given open connected sets $\Omega \subset \hat{\Omega} \subset \mathbb{C}^n$, we say that $\hat{\Omega}$ is the **analytic completion** or **holomorphy envelope** of Ω if and only if:

(i) $\hat{\Omega}$ is a holomorphy domain;
(ii) every function analytic in Ω has a continuation to all of $\hat{\Omega}$.

With this definition, not every open connected set will have an analytic completion, although if one extends the definition to allow $\hat{\Omega}$ to have a multisheeted structure, then every Ω does have a unique analytic completion. In the example above D_1 is the analytic completion of $D_1 \backslash \bar{D}_{\frac{1}{2}}$. We have already seen that D_1 obeys property (ii). To see that (i) holds, we note:

Proposition If $\Omega \subset \mathbb{C}^n$ is an open, connected, convex set, then Ω is a holomorphy domain.

Proof Given $w \notin \Omega$, we can find (by the Hahn–Banach theorem) a real linear functional ℓ from $\mathbb{C}^n \to \mathbb{R}$ so that $\ell(w) > \ell(z)$ for all $z \in \Omega$. Let

$$L(z) = \ell(z) - i\ell(iz)$$

and $f(z) = (L(z) - L(w))^{-1}$. Then f is analytic on Ω since $\operatorname{Re} L(z) \neq \operatorname{Re} L(w)$ for $z \in \Omega$, but f is singular at w. ∎

Paley–Wiener ideas are useful in discussing the analytic completions of certain special domains.

Definition Let $S \subset \mathbb{R}^n$ be open. The **tube over** S, denoted by $\mathcal{T}(S)$, is defined by:

$$\mathcal{T}(S) = \{x + iy | x \in \mathbb{R}^n, y \in S\}$$

Theorem IX.14.1 (Bochner's tube theorem) Let $S \subset \mathbb{R}^n$ be open and let $\hat{S}$ be its (open) convex hull. Then $\mathcal{T}(\hat{S})$ is the analytic completion of $\mathcal{T}(S)$.

Sketch of Proof It follows from the proposition that each $\mathcal{T}(\hat{S})$ is a holomorphy domain, so it suffices to show property (i). We shall sketch a proof of the slightly weaker fact that any polynomially bounded function $f(z)$ on $\mathcal{T}(S)$ extends to $\mathcal{T}(\hat{S})$. Since we could replace f by, for eaxmple, $e^{-z^2}f(z)$, this is not really much of a restriction, and one can recover the full result from this special case. By translating, we can suppose, without loss, that $0 \in S$. Let $g_y(x) = f(x + iy)$. For each $y \in S$, g_y is a tempered distribution, so let $T_y = \check{g}_y$. By the Paley–Wiener method, $T_y(x) = e^{x \cdot y}T_0(x)$. Thus T_0 is a tempered distribution with $e^{x \cdot y}T_0(x)$ tempered for all $y \in S$. By the lemma below, this is true for all $y \in \hat{S}$ and thus, turning the Paley–Wiener argument around, $\hat{T}_0$ is analytic in $\mathcal{T}(\hat{S})$. ∎

Lemma Let $T \in \mathcal{S}'(\mathbb{R}^n)$. Then the set of y so that $e^{x \cdot y}T(x) \in \mathcal{S}'(\mathbb{R}^n)$ is a convex set.

Proof Since convexity is defined in terms of line segments, it is not hard to see that it suffices to show that if T and $e^{\lambda}T(\lambda)$ are in $\mathcal{S}'(\mathbb{R})$, then $e^{\theta\lambda}T(\lambda)$ is in $\mathcal{S}'(\mathbb{R})$ for all $\theta \in (0, 1)$. Let φ_n be the nth Hermite function of the Appendix to Section V.3 (where the sequence space representation of $\mathcal{S}$ and $\mathcal{S}'$ is discussed). Define

$$g_n(z) = \int T(\lambda)e^{iz\lambda}\varphi_n(\lambda)\, d\lambda$$

which is entire since $e^{iz\lambda}\varphi_n(\lambda) \in \mathcal{S}$. Since T, $e^{\lambda}T(\lambda) \in \mathcal{S}'$, we have that

$$|g_n(x)| \leq C(1 + n^2)^m(2 + x^2)^m$$

$$|g_n(x - i)| \leq C(1 + n^2)^m(2 + x^2)^m$$

for suitable C and m. Applying the maximum principle to $(2 + z^2)^{-m-1}g_n(z)$, we see that $|g_n(-i\theta)| \leq D(1 + n^2)^m$ for all θ in $(0, 1)$ so $e^{\theta\lambda}T(\lambda) \in \mathcal{S}'$. ∎

This method is ideal for dealing with certain "degenerate cases." In the result below the reader should keep in mind the case $S = \{\langle y_1, y_2\rangle | y_1 = 0 \text{ or } y_2 = 0; |y_1| + |y_2| < 1\}$, which is *not* an open set.

(b) Use the Plancherel theorem to prove $c = 1/\sqrt{\alpha}$.
(c) Check the Fourier inversion formula explicitly in this example.

6. Let $\mathscr{H} = L^2(\mathbb{R}, e^{-x^2}\,dx)$ and define $\psi_n = x^n \in \mathscr{H}$ for $n = 0, 1, \ldots$.
(a) Prove that $\sum_{m=0}^{M} ((ik)^m/m!)\psi_m \xrightarrow[M\to\infty]{} e^{ikx}$ in the norm topology on $\mathscr{H}$.
(b) Suppose $\eta \in \mathscr{H}$ and $(x^m, \eta) = 0$ for all m. Prove $\varphi = 0$. (*Hint*: show that $\eta e^{-x^2} = 0$.)
(b′) Reach the conclusion of (b) without recourse to the Fourier transform. (*Hint*: Use the fact that the functions $(x \pm i)^{-n}$ are total in $C_\infty(\mathbb{R})$ and the formula $(x + i)^{-1} = i\int_0^\infty e^{-s}e^{isx}\,ds$).
(c) Let $\{H_n\}$ be the orthonormal set obtained from $\{\psi_n\}$ by Gram–Schmidt orthogonalization. Prove that $\{H_n\}$ is a basis for $\mathscr{H}$.
(d) Prove that $\{H_n(x)e^{-x^2/2}\}_{n=0}^{\infty}$ is an orthonormal basis for $L^2(\mathbb{R}, dx)$.
(e) Prove that $H_n(x)e^{-x^2/2}$ is just the nth Hermite function (defined in the Appendix to Section V.3).

7. Let $\{A_n(\lambda)\}$ be the polynomials determined by the formula

$$\sum_{n=0}^{\infty} A_n(\lambda)\frac{\alpha^n}{n!} = e^{-\alpha^2 + 2\alpha\lambda}$$

Define $\phi_n(\lambda) = (2^n n!)^{-1/2}A_n(\lambda)e^{-\lambda^2/2}$.
(a) Prove that

$$\phi_n(\lambda) = \frac{(-1)^n}{\sqrt{2^n n!}}\, e^{\lambda^2/2}\left(\frac{d}{d\lambda}\right)^n e^{-\lambda^2}$$

so that the $\phi_n(\lambda)$ are just the Hermite functions of the Appendix to Section V.3.
(b) If $f \in L^2(\mathbb{R}, dx)$ and $(f, \phi_n) = 0$ for all $n = 0, 1, \ldots$, prove that for all a,

$$\int f(x)e^{-(x-a)^2/2}\,dx = 0$$

(c) Use the Fourier transform to show that if $\int_{\mathbb{R}} f(x)e^{-(x-a)^2/2}\,dx = 0$ for all a, then $f = 0$.
(d) Conclude that $\{\phi_n\}$ is a basis for $L^2(\mathbb{R}, dx)$.

8. The purpose of this problem is to prove the Plancherel theorem and the inversion formula by using the Hermite functions. Let

$$A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right) \quad \text{and} \quad A^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)$$

(a) If $f \in \mathscr{S}(\mathbb{R}^n)$ prove $\widehat{A^\dagger f}(\lambda) = -i(A^\dagger \hat{f})(\lambda)$.
(b) Prove that $\hat{\phi}_n = (-i)^n\phi_n$.
(c) Supposing the fact that the Hermite functions are a basis for $L^2(\mathbb{R})$, prove the Plancherel theorem and the inversion formula.

9. Suppose that C is a continuous map of $\mathscr{S}(\mathbb{R}^n)$ into $C^\infty(\mathbb{R}^n)$ which commutes with translations. Prove that there is a $T \in \mathscr{S}'(\mathbb{R}^n)$ so that $C(\varphi) = T * \varphi$, for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$. (*Hint*: If $T \in \mathscr{S}'(\mathbb{R}^n)$ and $\varphi \in \mathscr{S}(\mathbb{R}^n)$, then $T(\varphi) = (T * \tilde{\varphi})(0)$.)

10. Prove directly (without using the Fourier transform) that for fixed $f \in \mathscr{S}(\mathbb{R}^n)$, the map $g \mapsto f * g$ is a continuous linear transformation of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$.

11. Let μ_1 and μ_2 be finite Borel measures on $\mathbb{R}^n$ and define

$$(\mu_1 * \mu_2)(E) = \int_{\mathbb{R}^n} \mu_1(E - y)\, d\mu_2(y)$$

(a) Prove that $\mu_1 * \mu_2$ is a finite Borel measure on $\mathbb{R}^n$, that $\mu_1 * \mu_2 = \mu_2 * \mu_1$, and that for any $f \in C_\infty(\mathbb{R}^n)$

$$(\mu_1 * \mu_2)(f) = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(x + y)\, d\mu_1(x)\, d\mu_2(y)$$

(b) Prove that $\mu_1 * \mu_2$ is absolutely continuous with respect to Lebesgue measure if either μ_1 or μ_2 is absolutely continuous with respect to Lebesgue measure. Give an example where $\mu_1 * \mu_2$ is not absolutely continuous.

12. The Fourier transforms of Borel measures of mass one on $\mathbb{R}^n$ are sometimes called "characteristic functions." A characteristic function $E(\lambda)$ is said to be **infinitely divisible** if for all positive integers n, there exists a characteristic function $E_n(\lambda)$ so that $E(\lambda) = (E_n(\lambda))^n$.

(a) Let μ be a Borel measure of mass one on $\mathbb{R}$ and let E be the corresponding characteristic function. Prove that E is infinitely divisible if and only if for all n there is a Borel measure of mass one, μ_n, so that

$$\mu = \underbrace{\mu_n * \mu_n * \cdots * \mu_n}_{n \text{ times}}$$

(b) Show that

$$E(\lambda) = \exp(i\alpha\lambda - \tfrac{1}{2}\beta\lambda^2) + \int_{-\infty}^{\infty} (e^{i\lambda x} - 1)\, d\rho$$

is an infinitely divisible characteristic function if $\alpha \in \mathbb{R}$, $\beta \geq 0$, and ρ is a Borel measure of finite mass on $\mathbb{R}$. Give a (convolution) formula for the corresponding measure in terms of α, β, and ρ. What is the corresponding measure if $\rho = 0$? What is the corresponding measure if $\alpha = 0 = \beta$ and $\rho = \delta(x - x_0)$?

Remark: There is a characterization of the Fourier transforms of all infinitely divisible distributions known as the Lévy–Khinchin formula. See, for example, L. Breiman, *Probability*, Addison Wesley, Reading, Massachusetts, 1968, 193–195.

13. Let Ω be an open set in $\mathbb{R}^n$, K a compact subset of Ω. Prove that there is a function in $C_0^\infty(\Omega)$ which is equal to one on K. (*Hint*: See Problem 61 of Chapter V.)

14. The purpose of this exercise is to prove the Fourier inversion formula by an alternative method. Suppose that $f \in \mathscr{S}(\mathbb{R}^n)$.

(a) Prove that $\lim_{\varepsilon \downarrow 0} \int_\varepsilon^{1/\varepsilon} ((\sin x)/x)\, dx$ exists. Call it d. Now, show that

$$\lim_{\varepsilon \downarrow 0} \int_\varepsilon^{1/\varepsilon} \frac{\sin Rx}{x}\, dx = d \qquad \text{for any } R > 0$$

(*Hint*: Use facts about telescoping series.)

(b) Prove that

$$\int_0^\infty \left[\frac{f(y-u)+f(y+u)}{2} - f(y)\right] \frac{\sin Ru}{u}\, du \xrightarrow[R\to\infty]{} 0$$

(Use the Riemann–Lebesgue lemma.)

(c) Using (b) conclude that

$$4df(y) = \lim_{R\to\infty} \int_{-\infty}^{\infty} \left(\int_{-R}^{R} e^{i(y-x)\cdot k} f(k)\, dk \right) dx$$

(d) Prove that $f(y) = (\sqrt{2\pi}/4d) \int_{-\infty}^{\infty} e^{iky} \hat{f}(y)\, dk$.

(e) By letting $f(x) = e^{-x^2/2}$, conclude that $d = \pi/2$.

15. The purpose of this exercise is to provide an alternative proof of the Plancherel theorem.

(a) Prove directly that if $f, g \in \mathscr{S}(\mathbb{R}^n)$

$$\widehat{f * g} = (2\pi)^{n/2} \hat{f}\hat{g}$$

(b) Letting $\tilde{f}(x) = f(-x)$, prove that

$$(f * \tilde{\bar{f}})(y) = \int |\hat{f}(k)|^2 e^{iky}\, dk$$

(c) Set $y = 0$ and conclude that

$$\int |f(x)|^2\, dx = \int |\hat{f}(k)|^2\, dk$$

***16.** Prove that the map $L^1(\mathbb{R}^n) \xrightarrow{\wedge} C_\infty(\mathbb{R}^n)$ is not onto by exhibiting a function in $C_\infty(\mathbb{R}^n)$ which is not in its range.

17. **The purpose of this problem is to develop the Fourier transform on $L^1(\mathbb{R}^n)$ without** reference to $\mathscr{S}(\mathbb{R}^n)$.

(a) If $f \in L^1(\mathbb{R}^n)$, prove directly that

$$\hat{f}(\lambda) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i\lambda x} f(x)\, dx$$

is a bounded continuous function. (*Hint*: Use the dominated convergence theorem.)

(b) If $f \in L^1(\mathbb{R}^n)$, prove that $\hat{f}(\lambda) \to 0$ as $|\lambda| \to \infty$. (*Hint*: Prove that $2\hat{f}(\lambda) = (2\pi)^{-n/2} \int e^{-ix\lambda}(f(x) - f(x - \pi\lambda/|\lambda|^2))\, dx$.

(c) Prove directly that $(2\pi)^{n/2} \hat{f}\hat{g} = \widehat{f * g}$.

18. Find a function $f(x)$ that satisfies all the conditions in the definition of "functions of positive type" except continuity. To which function of positive type is $f(x)$ equal a.e.?

19. Display a distribution of positive type that is not a function. What is its Fourier transform?

***20.** Prove the Bochner–Schwartz theorem (Theorem IX.10). (*Hint*: Mimic our proof of Bochner's theorem using the inner product $(\varphi, \psi) = T(\tilde{\bar{\varphi}} * \psi)$ and the formula $T(\tilde{\bar{\varphi}} * \varphi_x) = (T * \bar{\varphi} * \tilde{\varphi})(x)$.)

21. What does the generalization of the Paley–Wiener theorem to distributions with compact support say about the Fourier transform of distributions with support at the origin? Compute the same result directly by using Theorem V.11.

22. Let C be a convex, compact, balanced set in $\mathbb{R}^n$. Let

$$C^\circ = \{k \mid k \cdot x \geq -1 \text{ for all } x \in C\}$$

be its polar. Let ρ be the Minkowski functional of C°, i.e.,

$$\rho(\eta) = \sup_{x \in C}(\eta \cdot x) = \inf_{\lambda > 0}\{\lambda \mid \lambda \in \mathbb{R},\ \lambda\eta \in C^\circ\}$$

Prove the following version of the Paley–Wiener theorem:

A function $f \in \mathcal{S}(\mathbb{R}^n)$ has support in C if and only if $\hat{f}$ is the restriction to $\mathbb{R}^n$ of an entire function $\hat{f}(z)$ which obeys the condition that for any n there is a constant D_n so that

$$|\hat{f}(z)| \leq D_n(1 + |z|^2)^{-n} e^{-\rho(\operatorname{Im} z)}$$

Supplementary Material

Supplement to II.2 Applications of the Riesz lemma

There are a number of applications of the Riesz lemma (Theorem II.4) illustrating the power of abstract methods.

Application 1 (Von Neumann's proof of the Radon–Nikodym theorem) The following result implies both the Radon–Nikodym theorem (Theorem I.19) and the Lebesgue decomposition theorem (Theorem I.20) when all of the underlying measures are finite. To go from the finite to the σ-finite case is not hard (Problem 1).

Theorem S.1 Let μ and ν be finite measures on a measure space $\langle M, \mathscr{R} \rangle$. Then, there exists a set $A \in \mathscr{R}$ with $\nu(M \setminus A) = 0$ and $f \in L^1(M, d\nu)$ so that $f \geq 0$ and

$$\mu(B) = \int_B f(x)\, d\nu(x)$$

for all $B \subset A$.

Proof Let α be the measure $\mu + \nu$. Define the linear functional L on $L^2(M, d\alpha)$ by

$$L(g) = \int g \, d\mu$$

By the Schwarz inequality,

$$|L(g)| \leq \left(\int |g|^2 \, d\mu \right)^{\frac{1}{2}} \mu(M)^{\frac{1}{2}}$$

$$\leq \left(\int |g|^2 \, d\alpha \right)^{\frac{1}{2}} \mu(M)^{\frac{1}{2}}$$

so L is a bounded linear functional on $L^2(M, d\alpha)$. Thus, by the Riesz lemma, there is a function F with

$$\mu(C) = L(\chi_C) = \int_C F(x) \, d\alpha(x) \tag{S.1}$$

Fix $\gamma > 1$ and let $C_\gamma = \{x | F(x) \geq \gamma\}$. Then, by (S.1),

$$\mu(C_\gamma) \geq \gamma(\mu(C_\gamma) + \nu(C_\gamma))$$

from which it follows that

$$\mu(C_\gamma) = \nu(C_\gamma) = 0$$

so that $F \leq 1$ a.e. (with respect to α, μ, and ν). Since (S.1) holds with ν replacing μ and $1 - F$ replacing F, we see that $F \geq 0$ a.e. also.

Let

$$A_n = \{x | 1 - n^{-1} \leq F(x) < 1 - (n + 1)^{-1}\}$$

and

$$A = \bigcup_{n=1}^{\infty} A_n$$

Then, since $F(x) = 1$ on $M \backslash A$,

$$\mu(M \backslash A) = \int_{M \backslash A} F \, d\alpha = \mu(M \backslash A) + \nu(M \backslash A)$$

so $\nu(M \backslash A) = 0$.

Define $g_n(x) = F(x)(1 - F(x))^{-1}$ for $x \in A_n$, and $g_n(x) = 0$ for $x \notin A_n$. Then for any B and $h = \chi_B$, the characteristic function of B,

$$\begin{aligned}\int g_n h \, dv &= \int hF(1 - F)^{-1}\chi_{A_n}(1 - F)\, d\alpha \\ &= \int hF\chi_{A_n}\, d\alpha = \int h\chi_{A_n}\, d\mu \\ &= \mu(B \cap A_n)\end{aligned}$$

Taking $B = M$, we see that $\sum_{n=0}^{\infty} \int g_n \, dv = \mu(A) < \infty$, so $f = \sum_{n=0}^{\infty} g_n$ is in L^1 by the monotone convergence theorem. Moreover, if $B \subset A$,

$$\int_B f \, dv = \sum_n \int g_n h \, dv = \sum_n \mu(B \cap A_n) = \mu(B) \quad \blacksquare$$

Application 2 (the Bergmann reproducing kernel) Let Ω be a bounded open subset of $\mathbb{C}$. We want to introduce a natural object associated with the analytic structure of Ω. Write $z = x + iy$ and let $d^2z = dx\, dy$. Let $\mathscr{A}(\Omega)$ be the set of functions $f \in L^2(\Omega, d^2z)$ that are analytic in Ω.

Lemma For all $f \in \mathscr{A}(\Omega)$ and $z \in \Omega$,

$$|f(z)| \leq \pi^{-\frac{1}{2}}[\operatorname{dist}(z, \partial\Omega)]^{-1}\|f\|_2 \tag{S.2}$$

and $\mathscr{A}(\Omega)$ is a closed subset of $L^2(\Omega)$.

Proof First, suppose $\Omega = \{z \mid |z| < 1\}$. Then, by the Cauchy integral formula,

$$f(0) = \frac{1}{2\pi}\int_0^{2\pi} f(re^{i\theta})\, d\theta$$

for any $r < 1$. It follows that

$$\begin{aligned}|f(0)| &= \frac{1}{\pi}\left|\int_0^1 \int_0^{2\pi} f(re^{i\theta}) r \, dr \, d\theta\right| \\ &\leq \|f\|_2 \pi^{-1}\pi^{\frac{1}{2}} = \pi^{-\frac{1}{2}}\|f\|_2\end{aligned}$$

By scaling and translation, if $\{z \mid |z - z_0| < r\} \subset \Omega$, then

$$|f(z_0)| \leq \pi^{-\frac{1}{2}} r^{-1}\|f\|_2$$

so that (S.2) follows.

(S.2) implies that whenever $f_n \to f$ in L^2 and $f_n \in \mathscr{A}$, then f_n converges to f uniformly on compact subsets of Ω. Therefore, by a theorem of Weierstrass (which follows from the Cauchy integral formula), f is in $\mathscr{A}$. ∎

Theorem S.2 Let Ω be a bounded open subset of $\mathbb{C}$. Then, there exists a function $K(z, w)$ on $\Omega \times \Omega$ so that:

(a) K is analytic in z and $\overline{w}$
(b) $|K(z, w)| \leq \pi^{-1}[\text{dist}(z, \partial\Omega)]^{-1}[\text{dist}(w, \partial\Omega)]^{-1}$
(c) $\overline{K(z, w)} = K(w, z)$
(d) For any fixed z, $\overline{K(z, w)} \in \mathscr{A}(\Omega)$
(e) For any $f \in \mathscr{A}(\Omega)$

$$f(z) = \int_\Omega K(z, w) f(w)\, d^2w \tag{S.3}$$

Proof By the lemma, $\mathscr{A}(\Omega)$ is a Hilbert space. By (S.2), $f \to f(z)$ is a bounded linear functional on $\mathscr{A}$ for each fixed $z \in \Omega$. So, by the Riesz lemma, there exists $h_z \in \mathscr{A}(\Omega)$ such that

$$f(z) = (h_z, f) \tag{S.4}$$

for any $f \in \mathscr{A}$ and

$$\|h_z\| \leq \pi^{-\frac{1}{2}}[\text{dist}(z, \partial\Omega)]^{-1} \tag{S.5}$$

Let P be the orthogonal projection from $L^2(\Omega)$ to $\mathscr{A}(\Omega)$ (projections are defined in Section VI.2, but their existence depends only on Theorem II.3). Since $h_z \in \mathscr{A}$, for any $g \in L^2$,

$$(h_z, g) = (Ph_z, g) = (h_z, Pg) = (Pg)(z)$$

It follows (using Theorem VI.4) that $z \to h_z$ is antianalytic in z. Now define

$$K(z, w) = (h_z, h_w)$$

Using (S.5) and the above, (a)–(c) are obvious. Moreover, by (S.4),

$$K(z, w) = \overline{(h_w, h_z)} = \overline{h_z(w)}$$

so (d) is evident and (S.4) implies (S.3). ∎

Because of (S.3), K is called the **Bergmann reproducing kernel** for Ω.

Example Let $\{g_n(z)\}_{n=0}^{\infty}$ be an orthonormal basis for $\mathcal{A}(\Omega)$ (orthonormal bases are defined in Section II.3). Then

$$K(z, w) = \sum_{n=0}^{\infty} (h_z, g_n)(g_n, h_w)$$

$$= \sum_{n=0}^{\infty} g_n(z)\overline{g_n(w)} \tag{S.6}$$

By Theorem II.6, the expression (S.6) converges to $K(z, w)$ for each fixed z and w. But, since the finite sums are uniformly bounded on compact subsets and analytic in z and $\bar{w}$, the Vitali convergence theorem implies that (S.6) is uniformly convergent on compact subsets of Ω.

Consider the case $\Omega = \{z : |z| < 1\}$. Then $\{z^n(2n + 2)^{\frac{1}{2}}(2\pi)^{-\frac{1}{2}}\}_{n=0}^{\infty}$ is an orthonormal set, and it is not hard to see that it is a basis (Problem 2). Thus, by (S.6),

$$K(z, w) = \sum_{n=0}^{\infty} \pi^{-1}(n + 1)(z\bar{w})^n = \pi^{-1}(1 - z\bar{w})^{-2}$$

in the case where Ω is the unit disk.

Supplement to III.1 Basic properties of L^p spaces

In this supplement we prove some of the basic facts about L^p spaces which are presented without proof in Sections III.1 and III.2.

Theorem S.3 (Hölder's inequality) Let $1 < p < \infty$, $p^{-1} + q^{-1} = 1$. Let $f \in L^p$, $g \in L^q$. Then $fg \in L^1$ and

$$\|fg\|_1 \leq \|f\|_p \|g\|_q \tag{S.7}$$

Moreover, if neither f nor g are a.e. zero, equality holds in (S.7) if and only if $|g|$ is a.e. a constant multiple of $|f(x)|^{p-1}$.

Proof We begin by proving an inequality on positive numbers:

$$ab \leq a^p p^{-1} + b^q q^{-1} \tag{S.8}$$

To prove this, consider the graph of the function

$$a = F(b) \equiv b^{q-1}$$

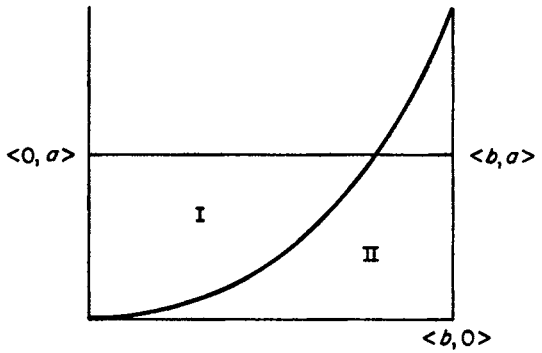

FIGURE S.1 The graph of $a = b^{q-1}$, $b = a^{p-1}$.

or equivalently

$$b = F^{-1}(a) = a^{p-1}$$

since $(p-1)(q-1) = 1$. (S.8) is geometrically obvious from Figure S.1: for the area of region I is clearly equal to $\int_0^a a^{p-1}\,da = a^p/p$ and the area of region II is less than $\int_0^b b^{q-1}\,db = b^q/q$.

Now we can prove (S.7). It is easy to prove if f or g is a.e. zero. By replacing f by $f\|f\|_p^{-1}$ and g by $g\|g\|_q^{-1}$, we need only prove (S.7) when $\|f\|_p = \|g\|_q = 1$. Then, by (S.8),

$$\int |f(x)g(x)|\,dx \le p^{-1}\int |f(x)|^p\,dx + q^{-1}\int |g(x)|^q\,dx$$

$$= p^{-1} + q^{-1} = 1$$

This proves (S.7). That equality holds when $|g(x)| = |f(x)|^{p-1}$ is easy. That it only holds in this case is left to the reader (Problem 4). ∎

Corollary 1 Let $f \in L^p$, $1 \le p \le \infty$. Then

$$\|f\|_p = \sup\{\|fg\|_1 \mid \|g\|_q = 1\} \tag{S.9}$$

Proof. That $\|f\|_p$ is greater than or equal to the sup follows from (S.7). To get equality, take g to be a suitable multiple of $|f(x)|^{p-1}$. ∎

Corollary 2 (Minkowski's inequality) Let $1 \le p \le \infty$. Then

$$\|f+g\|_p \le \|f\|_p + \|g\|_p$$

Proof By (S.9) and the triangle inequality for $\|\cdot\|_1$,

$$\begin{aligned}\|f+g\|_p &= \sup\{\|(f+g)h\|_1 \mid \|h\|_q = 1\} \\ &\le \sup\{\|fh\|_1 + \|gh\|_1 \mid \|h\|_q = 1\} \\ &\le \sup\{\|fh\|_1 \mid \|h\|_q = 1\} + \sup\{\|gh\|_1 \mid \|h\|_q = 1\} \\ &= \|f\|_p + \|g\|_p \quad \blacksquare\end{aligned}$$

Theorem S.4 Let $\langle X, \mu\rangle$ be a σ-finite measure space, $1 \le p < \infty$, and L be an element of $L^p(X, d\mu)^*$. Then there exists $g \in L^q(X, d\mu)$ with $\|g\|_q = \|L\|_{(L^p)^*}$ so that

$$L(f) = \int g(x)f(x)\,d\mu(x) \tag{S.10}$$

Thus $(L^p)^*$ is isometrically isomorphic to L^q.

Proof By Theorem S.3, the L in (S.10) is a bounded linear functional on L^p if $g \in L^q$ with norm $\|L\|_{(L^p)^*} \le \|g\|_q$. In fact, $\|L\|_{(L^p)^*} = \|g\|_q$ by Corollary 1. Thus, we need only prove the existence of g, given L.

Suppose that $\mu(X) < \infty$ and that we are given an $L \in (L^p)^*$ which is **positive** in the sense that $L(f) \ge 0$ for $f \ge 0$. Define a function ν on measurable sets by

$$\nu(A) = L(\chi_A)$$

where χ_A is the characteristic function of A. Since $p < \infty$, if $A = \bigcup_{n=1}^{\infty} A_n$ with A_i disjoint, then $\sum_{n=0}^{N} \chi_{A_n} \to \chi_A$ in L^p by the monotone convergence theorem. Thus

$$\nu(A) = \lim_{N\to\infty} L\left(\sum_{n=1}^{\infty} \chi_{A_n}\right) = \sum_{n=1}^{\infty} \nu(A_n)$$

so ν defines a measure. If $\mu(A) = 0$, then $\chi_A = 0$ in L^p so $\nu(A) = 0$. Therefore, by the Radon–Nikodym theorem, there exists $g \in L^1$ with $g \ge 0$ so that

$$L(\chi_A) = \int g(x)\chi_A(x)\,d\mu(x)$$

for any A. Now let h be bounded and positive. One can find h_n so that $h_n(x) \uparrow h(x)$, $\|h_n - h\|_p \to 0$, and each h_n is a finite linear combination of χ_A's. Thus, by the monotone convergence theorem,

$$L(h) = \int h(x)g(x)\,d\mu(x)$$

Fix K and let $h(x) = |g(x)|^{q-1}$ (resp. 0) if $|g(x)| \leq K$ (resp. $|g(x)| > K$). Then

$$\int_{|g(x)| \leq K} |g(x)|^q \, d\mu(x) = L(h) \leq \|L\| \left(\int_{|g(x)| \leq K} |g(x)|^{(q-1)p} \, d\mu(x) \right)^{1/p}$$

$$= \|L\| \left(\int_{|g(x)| \leq K} |g(x)|^q \, d\mu(x) \right)^{1-1/q}$$

Therefore,

$$\int_{|g(x)| \leq K} |g(x)|^q \, d\mu(x) \leq \|L\|^q$$

Since $\|L\| < \infty$, and g is a.e. finite, we conclude that $g \in L^q$.

This proves the result if L is positive and $\mu(X) < \infty$. The argument in the proof of Theorem IV.16 shows that any $L \in (L^p)^*$ is a finite linear combination of positive L's (Problem 6), and it is also easy to extend the result to the σ-finite case (Problem 7). ∎

Supplement to IV.3 Proof of Tychonoff's theorem

In this supplement we provide a proof of Tychonoff's theorem, Theorem IV.5, fleshing out the proof sketched in the notes to Section IV.3.

Definition A net $\{x_\alpha\}_{\alpha \in I}$ of points in some set X is called a **universal net** if and only if for *every* subset $A \subset X$ either eventually $x_\alpha \in A$ or else eventually $x_\alpha \in X \setminus A$.

Notice that the notion of universal net makes no mention of topology. Also notice that this is a very strange notion. For example, the sequence $\{x_n = 1/n\}$ is not universal, for suppose that $A = \{1/2n\}$. In fact, no *sequence* which is not eventually constant is a universal net (Problem 8). The point of the definition is the following obvious result.

Lemma 1 Any cluster point of a universal net is the limit of the net.

Universal nets are so strange that it is not clear that any exist. Indeed, the existence of a universal subnet for the sequence $\{x_n = n\}_{n \in \mathbb{Z}}$ is equivalent to the axiom of choice. Using this axiom, we can construct lots of universal nets.

The questions of the uniqueness of α and the positivity of $d\alpha$ if L is positive are left to the reader (Problems 9 and 10). Our proof is very special in that it does not extend naturally to more general spaces. We give it for two reasons: Most applications that we give, in particular the spectral theorem, require only the case $X = [0, 1]$ or the case $X = (-\infty, \infty)$ which is a simple extension. Secondly, the proof is a nice illustration of the power of the Hahn–Banach theorem.

Proof of Theorem S.5 Let $PC_{\mathbb{R}}[0, 1]$ be the space defined in Section I.2. By the Hahn–Banach theorem, L extends to a bounded linear functional $\tilde{L}$ on $PC_{\mathbb{R}}[0, 1]$. Let $\chi_{[x,y)}$ denote the characteristic function of $[x, y)$. Define

$$\alpha(x) = \tilde{L}(\chi_{[0,x)}) \qquad \text{if} \quad x < 1$$
$$\alpha(1) = \tilde{L}(\chi_{[0,1]})$$

We first claim that α is of bounded variation. Fix $0 = x_0 < x_1 < \cdots < x_n = 1$ and let $\chi_i = \chi_{[x_{i-1}, x_i)}$ except for $i = n$, for which we take $\chi_n = \chi_{[x_{n-1}, x_n]}$. Then, for any $a_1, \ldots, a_n \in \mathbb{R}$,

$$\begin{aligned} |\textstyle\sum a_i[\alpha(x_i) - \alpha(x_{i-1})]| &= |\tilde{L}(\textstyle\sum a_i \chi_i)| \\ &\le \|\tilde{L}\| \sup_i |a_i| \end{aligned}$$

From this it follows that

$$\sum |\alpha_i(x_i) - \alpha(x_{i-1})| \le \|\tilde{L}\|$$

by taking each $a_i = \pm 1$. Thus α has bounded variation.

Now, given $f \in C[0, 1]$, let $\chi_i^{(n)}$ be the above functions for $x_i = i/n$ and let

$$f_n = \sum_{i=1}^{n} f\left(\frac{i}{n}\right)\chi_i^{(n)}$$

Then, $f_n \xrightarrow{PC[0,1]} f$. Moreover, $\tilde{L}(f_n) = \int f_n \, d\alpha$ by construction. Thus

$$L(f) = \lim_n \tilde{L}(f_n) = \lim_n \int f_n \, d\alpha = \int f \, d\alpha \qquad \blacksquare$$

Supplement to IV.5 Minimization of functionals

In this supplement we want to show how the Banach–Alaoglu theorem can be used to prove that certain functionals on Banach spaces take on their minimum value. Such minimization problems often occur, for example, in

the problem of finding geodesics, i.e., curves of minimum length. They also enter in the context of solving equations of the form

$$T(u) = 0 \tag{S.11}$$

where T is a map from X to X^*. For suppose that T is the gradient of a map F from X to $\mathbb{R}$ in the sense that

$$\frac{d}{d\lambda} F(u + \lambda v)\Big|_{\lambda=0} = (T(u))(v)$$

Then, if u minimizes F, it obeys (S.11).

An attractive method for showing that a function takes its minimum value is to show that it is a continuous function on a compact set. For this, the norm topology is not usually suitable, since only rather small subsets of Banach spaces are compact in the norm topology. On the other hand, the Banach–Alaoglu theorem suggests that, when X is reflexive, the weak topology is an attractive possibility. The only problem with this is that lots of natural functions are *not* weakly continuous. For example, the norm is not weakly continuous for if it were, then $\{x \mid |x| = 1\}$ would be weakly closed and it is not (Problem 40 of Chapter IV). However, if $x_n \to x$ weakly, then

$$\begin{aligned} \|x\| &= \sup\{|\ell(x)| \mid \ell \in X^*;\ \|\ell\| = 1\} \\ &= \sup\{\lim |\ell(x_n)| \mid \ell \in X^*,\ \|\ell\| = 1\} \\ &\le \sup\{\underline{\lim}\|\ell\|\ \|x_n\|\} = \underline{\lim}\|x_n\| \end{aligned}$$

This shows that $\|\cdot\|$ is weakly lower semicontinuous where:

Definition A function F from a topological space X to $\mathbb{R}$ is called **lower semicontinuous** (l.s.c.) if and only if $x_\alpha \to x$ implies that $F(x) \le \underline{\lim}\ F(x_\alpha)$.

One can show (Problem 11) that F is l.s.c. if and only if $\{x \mid F(x) \le \alpha\}$ is closed for all α. The point of this definition is the following:

Proposition A lower semicontinuous function F on a compact space is bounded from below and takes its minimum value.

Proof Let $A = \inf_x F(x)$. If $A > -\infty$, pick x_n with

$$F(x_n) \le A + n^{-1}$$

Clearly, for every $A \subset X$, we must make a choice of either A or $X \setminus A$. These choices are not quite independent, since if x_α is eventually in both A and B, then it is eventually in $A \cap B$ so $A \cap B \neq \varnothing$. This motivates:

Definition A **filter** is a family $\mathcal{F}$ of subsets of X obeying:

(i) $\varnothing \in \mathcal{F}$;
(ii) if $A, B \in \mathcal{F}$, then $A \cap B \in \mathcal{F}$;
(iii) if $A \subset B$ and $A \in \mathcal{F}$, then $B \in \mathcal{F}$.

An **ultrafilter** is a maximal filter, i.e., a filter that is not strictly contained in any other filter.

Example 1 Fix x_0. Then $\{A \mid x_0 \in A\}$ is an ultrafilter.

Example 2 Let $\{x_\alpha\}_{\alpha \in I}$ be any net. Then $\mathcal{F} = \{A \mid x_\alpha \text{ is eventually in } A\}$ is a filter.

Lemma 2 Any filter is contained in an ultrafilter.

Proof A simple application of Zorn's lemma. ∎

The following lemma shows the connection between ultrafilters and universal nets.

Lemma 3 If $\mathcal{U}$ is an ultrafilter, then for any $A \subset X$, either $A \in \mathcal{U}$ or $X \setminus A \in \mathcal{U}$.

Proof Suppose that $\mathcal{F}$ is any filter and $B \subset X$ obeys $B \cap C \neq \varnothing$ for all $C \in \mathcal{F}$. Then $\{C \cap D \mid C \in \mathcal{F}, B \subset D\}$ is a filter containing $\mathcal{F}$ and B. Therefore, if $\mathcal{U}$ is an ultrafilter, and $B \notin \mathcal{U}$, then there is a $C \in \mathcal{U}$ with $B \cap C = \varnothing$.

Thus if $A \notin \mathcal{U}$ and $X \setminus A \notin \mathcal{U}$, we can find $C, D \in \mathcal{U}$ with $A \cap C = \varnothing$ and $(X \setminus A) \cap D = \varnothing$. Therefore,

$$\begin{aligned} C \cap D &= C \cap D \cap X \\ &= [(C \cap D) \cap A] \cup [(C \cap D) \cap (X \setminus A)] \\ &= \varnothing \end{aligned}$$

which is not allowed since C and D are in $\mathcal{U}$. Thus, to avoid contradiction, either $A \in \mathcal{U}$ or $X \setminus A \in \mathcal{U}$. ∎

The following lemma contains all the hard work in the proof of Tychonoff's theorem.

Lemma 4 Any net has a universal subnet.

Proof Let $\{x_\alpha\}_{\alpha \in I}$ be the net and let $\mathscr{U}$ be an ultrafilter containing the filter, $\mathscr{F}$ of Example 2. Let $J = \{\langle \alpha, A\rangle | \alpha \in I, A \in \mathscr{U}, x_\alpha \in A\}$. Order J by $\langle \alpha, A\rangle > \langle \beta, B\rangle$ if $\alpha > \beta$ and $A \subset B$. The following argument shows that J is directed: If $A \in \mathscr{U}$, then x_α is frequently in A for if it were not, then $X \setminus A \in \mathscr{F} \subset \mathscr{U}$. Thus, given any A, B, α, β, there is $\gamma > \alpha, \beta$ so that $x_\gamma \in A \cap B$, i.e., J is directed. Let $F: J \to I$ by $F(\alpha, A) = \alpha$. Then $y_{\langle \alpha, A\rangle} = x_\alpha$ is a subnet of $\{x_\alpha\}_{\alpha \in I}$. Moreover, given any $A \in \mathscr{U}$, find α with $x_\alpha \in A$. If $\langle \beta, B\rangle > \langle \alpha, A\rangle$, then $y_{\langle \beta, B\rangle} \in A$ so y is eventually in A. By Lemma 3, we conclude that y is a universal net. ∎

Lemma 5 A Hausdorff topological space X is compact if and only if all universal nets converge.

Proof If X is compact, then by the Bolzano–Weierstrass theorem, any universal net has a cluster point and so, by Lemma 1, a limit. Conversely, by Lemma 4, if all universal nets converge, then every net has a convergent subnet so X is compact by the Bolzano–Weierstrass theorem. ∎

Proof of Tychonoff's theorem (Theorem IV.5) Let $\{x^{(\beta)}\}_{\beta \in I}$ be a universal net in $X = \bigtimes X_\alpha$ where each X_α is compact. Then $\{x_\alpha^{(\beta)}\}_{\beta \in I}$ is universal in X_α, so by Lemma 5, $x_\alpha^{(\beta)} \to x_\alpha^{(\infty)}$ for some $x_\alpha^{(\infty)} \in X_\alpha$. Thus, there is $x^{(\infty)}$ in X with $x^{(\beta)} \to x^{(\infty)}$. By Lemma 5 again, X is compact. ∎

Supplement to IV.4 The Riesz–Markov theorem for $X = [0, 1]$

Functions of bounded variation and Riemann–Stieltjes integrals are defined in Problem 11 of Chapter 1. In this supplement we prove:

Theorem S.5 Let $L \in (C_{\mathbb{R}}[0, 1])^*$. Then, there exists a function α of bounded variation so that

$$L(f) = \int_0^1 f \, d\alpha$$

for any $f \in C_{\mathbb{R}}[0, 1]$.

and if $A = -\infty$, pick x_n with $F(x_n) \leq -n$. Let x be a cluster point of the x_n and let $x_{n(\alpha)}$ be a subnet converging to x. Then, by lower semicontinuity,

$$F(x) \leq \underline{\lim}\, F(x_{n(\alpha)}) = A$$

Thus $A \neq -\infty$ and $F(x) = A$. ∎

The Banach-Alaoglu theorem therefore implies the following basic result:

Theorem S.6 Let M be a weakly closed subset of a reflexive Banach space X. Suppose that F is a function from M to $\mathbb{R}$ obeying:

(i) for some a, $\{x \in M \mid F(x) \leq a\}$ is a *bounded* nonempty subset of X;
(ii) F is weakly lower semicontinuous.

Then, F is bounded from below and there exists $x_0 \in M$ with

$$F(x_0) = \min_{x \in M} F(x)$$

Notice that there are no changes in the above if we allow F to take the value $+\infty$. Henceforth we allow this.

It is important to have a large supply of weakly l.s.c. functions. The following is often useful:

Definition A function F on a vector space V is called **convex** if

$$F(\lambda x + (1 - \lambda)y) \leq \lambda F(x) + (1 - \lambda)F(y)$$

for all $x, y \in V$ and $\lambda \in [0, 1]$.

Theorem S.7 Let F be a function from a Banach space X to $(-\infty, \infty]$ (with $+\infty$ allowed). Suppose that $\{x \in X \mid F(x) < \infty\} = V$ is a subspace, that F is convex on V, and that F is norm l.s.c. Then F is weakly l.s.c.

Proof Since F is convex, $\{x \mid F(x) \leq a\}$ is convex. It is norm closed by Problem 11 since F is norm l.s.c. By general principles (Problem 12) such a set is weakly closed. Thus, by Problem 11 again, F is weakly l.s.c. ∎

Example 1 Let $G: \mathbb{C} \to [0, \infty)$ be convex and let $\langle M, \mu \rangle$ be a measure space. Then the functional

$$F(u) = \int G(u(x))\, d\mu(x)$$

(F may be $+\infty$) is weakly l.s.c. on all the L^p spaces, $p < \infty$. For F is clearly convex and therefore it suffices to prove that F is norm l.s.c. Let $u_n \to u$ in L^p norm. Pick a subsequence with $\lim_i F(u_{n(i)}) = \underline{\lim}\, F(u_n)$ and then a further subsequence so that $u_{n(i)}(x) \to u(x)$ pointwise a.e. Then $G(u_{n(i)}(x)) \to G(u(x))$ pointwise since a convex function is automatically continuous. So, by Fatou's lemma (Theorem I.17),

$$F(u) \leq \underline{\lim}\, F(u_{n(i)})$$

This establishes that F is weakly l.s.c. Notice that a special case of this example is the fact that the L^r norm is weakly l.s.c. on L^p for any p and $r < \infty$.

We want to sketch some applications of these ideas. Occasionally, we shall use terminology not defined until Chapter V or Volume II.

Example 2 (a nonlinear elliptic equation) Given a real-valued function $f \in C_0^\infty(\mathbb{R}^\nu)$, we shall show the existence of a real-valued function $u \in L^2(\mathbb{R}^\nu)$ such that

$$-\Delta u + u|u| + u = f \tag{S.12}$$

where $-\Delta u$ is interpreted in the sense of distributions. Once one knows that this equation has a solution in L^2, the regularity methods of Section IX.6 show that u is, in fact, C^3. To solve (S.12) we define $F : L^2 \to (-\infty, \infty]$ by

$$F(u) = \tfrac{1}{2}\int |\nabla u|^2\, dx + \tfrac{1}{3}\int |u|^3\, dx + \tfrac{1}{2}\int |u|^2\, dx - \int f(x)u(x)\, dx$$

where we set $F(u) = \infty$ if $u \notin L^3$ or if $\nabla u \notin L^2$. If $g \in C_0^\infty(\mathbb{R}^\nu)$ and $F(u) < \infty$, then $F(u + \lambda g)$ is differentiable in λ and

$$\frac{d}{d\lambda} F(u + \lambda g)\bigg|_{\lambda = 0} = \int g(x)[-\Delta u(x) + |u(x)|u(x) + u(x) - f(x)]\, dx$$

If u minimizes F, then the left-hand side is zero. Since this is true for all $g \in C_0^\infty$, u satisfies (S.12). Thus, we wish to show that F takes on its minimum value.

By the Schwarz inequality,

$$F(u) \geq \tfrac{1}{2}\|u\|_2^2 - \|u\|_2\|f\|_2 \geq \tfrac{1}{4}\|u\|_2^2 - \|f\|_2^2$$

Thus, $\{u \in L^2 \mid F(u) \leq 1\}$ is bounded, and it is nonempty since $F(0) = 0$. As a result, by Theorem S.6, it suffices to prove that F is weakly l.s.c. The last term is

obviously weakly continuous, and the second and third terms are weakly l.s.c. by Theorem S.7. As for the first term, let $u_n \to u$ weakly; then

$$\begin{aligned}
\|\nabla u\|_2 &= \sup\{|(f, \nabla u)| \mid f \in C_0^\infty, \|f\|_2 = 1\} \\
&= \sup\{|(\nabla \cdot f, u)| \mid f \in C_0^\infty, \|f\|_2 = 1\} \\
&\le \sup\left\{\liminf_n |(\nabla \cdot f, u_n)| \mid f \in C_0^\infty, \|f\|_2 = 1\right\} \\
&= \sup\left\{\liminf_n |(f, \nabla u_n)| \mid f \in C_0^\infty, \|f\|_2 = 1\right\} \\
&\le \liminf_n \|\nabla u_n\|_2
\end{aligned}$$

This proves the existence of solutions of (S.12).

The proof that we used above depends very strongly on the form of the nonlinear term $g(u) = (|u| + 1)u$. In particular, it depends on the fact that g is the derivative of a convex function. This is certainly necessary for the method to work. However, our proof above would not work if $g(u) = |u|u$, even though $|z|^3$ is convex, since we would not know that $\{u \mid F(u) \le 1\}$ is bounded in L^2. Also it would not work if $g(u) = u^3 + u$, for in that case we could not argue that $u \in L^2$ implies that $g(u)$ is a distribution (i.e., an L^1_{loc} function). However, both of these difficulties are easy to overcome (Problem 15) if one realizes that L^2 is not sacred. In fact, for $|g(u)| \le |u|^{p-1}$, the natural space to take is $L^p \cap H_1$ where $H_1 = \{u \in L^2 \mid \nabla u \in L^2\}$ with the norm $(\|\nabla u\|_2^2 + \|u\|_2^2)^{\frac{1}{2}}$. That this space is the dual space of $L^q + H_1^*$ follows from general principles (Problem 14).

Example 3 (the Thomas–Fermi equations) Fix $z_1, \ldots, z_k > 0$ and $\mathbf{R}_1, \ldots, \mathbf{R}_k \in \mathbb{R}^3$ and let

$$V(\mathbf{r}) = \sum_{i=1}^{k} z_i |\mathbf{r} - \mathbf{R}_i|^{-1}$$

The **Thomas–Fermi equations** are

$$\rho = \max(\varphi, 0)^{\frac{3}{2}}$$

$$\varphi(\mathbf{x}) = V(\mathbf{x}) - \int \rho(\mathbf{y}) |\mathbf{x} - \mathbf{y}|^{-1} \, d\mathbf{y} \tag{S.13}$$

Occasionally, this is written as the differential equation

$$-\Delta\varphi + 4\pi[\max(\varphi, 0)]^{\frac{3}{2}} = 4\pi \sum_{i=1}^{k} z_i \delta(r - R_i)$$

To solve this, we let

$$\mathscr{E}(\rho) \equiv \frac{3}{5}\int \rho^{\frac{5}{3}}(x)\,dx - \int V(x)\rho(x)\,dx + \frac{1}{2}\int \frac{\rho(x)\rho(y)}{|x-y|}\,dx\,dy \qquad \text{(S.14)}$$

defined on $\{\rho \mid \rho \in L^{\frac{5}{3}}, \rho \in K, \rho \geq 0\}$, where K is the completion of C_0^∞ in the norm

$$\|\rho\|_K \equiv \left(\int \frac{\rho(x)\rho(y)}{|x-y|}\,dx\,dy\right)^{\frac{1}{2}}$$

That the integral in question is positive follows from the fact that $\|\rho\|_K^2 = \lim_{a \downarrow 0} 4\pi(\rho, (-\Delta + a)^{-1}\rho)$. By general principles (Problem 14), $L^{\frac{5}{3}} \cap K$ is the dual space of the sum of functionals in $L^{\frac{5}{3}}$ and K^*. The first and third terms of (S.14) are weakly l.s.c. by general arguments (Theorem S.7). We leave it to the reader (Problem 16) to prove that the middle term is a linear functional in $L^{\frac{5}{3}} + K^*$. It follows that $\mathscr{E}(\rho)$ takes its minimum value and, as in Example 2, the minimizing ρ solves (S.13). The reason that $\max\{\varphi, 0\}$ enters is that we know that

$$\frac{d}{d\lambda}\mathscr{E}(\rho + \lambda g)\bigg|_{\lambda=0} = 0$$

only for g with $|g| \leq c\rho$. For general $g \geq 0$, we only know that

$$\frac{d}{d\lambda}\mathscr{E}(\rho + \lambda g)\bigg|_{\lambda=0} \geq 0$$

It can be proven using special features of this problem that $\varphi > 0$ if φ is the minimizing function (see the reference in the notes).

Example 4 (Hartree equations for helium) We seek solutions of the equations

$$\begin{aligned} -\Delta u - 2|x|^{-1}u + W_1(x)u &= \varepsilon_1 u \\ -\Delta v - 2|x|^{-1}v + W_2(x)v &= \varepsilon_2 v \end{aligned} \qquad \text{(S.15)}$$

$x \in \mathbb{R}^3$, with the subsidiary conditions

$$\|u\|_2 = \|v\|_2 = 1 \qquad \text{(S.16)}$$

and

$$W_1(x) = \int |x-y|^{-1}v(y)\,dy$$

$$W_2(x) = \int |x-y|^{-1}u(y)\,dy$$

The physical significance of the equations is that formally (S.15) comes from minimizing

$$\mathscr{E}(u, v) = \int (|\nabla u|^2 + |\nabla v|^2)\, dx - 2 \int |x|^{-1}(|u|^2 + |v|^2)$$

$$+ \int |u(x)|^2 |v(y)|^2 |x - y|^{-1}\, dx\, dy \tag{S.17}$$

with the subsidiary condition (S.16); the ε_i are just Lagrange multipliers. For u and v obeying (S.16), one sees that

$$\mathscr{E}(u, v) = (\psi, H\psi)$$

$$\psi(x, y) = u(x)v(y)$$

where

$$H = -\Delta_x - \Delta_y - \frac{2}{|x|} - \frac{2}{|y|} + \frac{1}{|x - y|}$$

so that solutions of (S.15), (S.16) can be expected to give approximate solutions of $H\psi = E\psi$ in some vague sense.

The new feature of this example is the subsidiary condition (S.16), for the set of functions obeying (S.16) is *not* weakly closed. Thus, once one shows that $\mathscr{E}$ is weakly lower semicontinuous on $H_1 \oplus H_1$ with $H_1 = \{u | \nabla u \in L^2, u \in L^2\}$ (see the reference in the Notes for this), one can use Theorem S.6 to show only that $\mathscr{E}$ takes its minimum subject to the subsidiary conditions

$$\|u\|_2 \leq 1, \qquad \|v\|_2 \leq 1 \tag{S.18}$$

for this set is the weak closure of the set obeying (S.16). However, one can actually show that the minimizing function subject to (S.18) obeys (S.16). For, let $u^{(0)}$ and $v^{(0)}$ minimize $\mathscr{E}$ subject to (S.18). Then

$$\mathscr{E}(u, v^{(0)}) = c + (u, hu)$$

where

$$h = -\Delta + V(x)$$

$$V(x) = -\frac{2}{|x|} + \int |v^{(0)}(y)|^2 |x - y|^{-1}\, dy$$

Let $\tilde{u}$ be the function that is the lowest eigenvector of $\tilde{h} = -\Delta - |x|^{-1}$. Then

$$(\tilde{u}, h\tilde{u}) = (\tilde{u}, \tilde{h}\tilde{u}) + (v^{(0)}, \tilde{W}v^{(0)})$$

where

$$\tilde{W}(x) = -|x|^{-1} + \int |\tilde{u}(y)|^2 |x - y|^{-1}\, dy$$

$$= -|x|^{-1} + \int |\tilde{u}(y)|^2 [\max\{|y|, |x|\}]^{-1}\, dy \leq 0$$

since $\tilde{u}$ is spherically symmetric. Thus

$$(\tilde{u}, h\tilde{u}) < 0$$

It follows that $(u^{(0)}, hu^{(0)}) < 0$, for if not, then we would have $\mathscr{E}(\tilde{u}, v^{(0)}) < \mathscr{E}(u^{(0)}, v^{(0)})$. If $\|u^{(0)}\|_2 = a$, then

$$\mathscr{E}(a^{-1}u^{(0)}, v^{(0)}) = \mathscr{E}(u^{(0)}, v^{(0)}) + (a^{-2} - 1)(u^{(0)}, hu^{(0)})$$

Since $\langle u^{(0)}, v^{(0)} \rangle$ minimizes $\mathscr{E}(u^{(0)}, v^{(0)})$ over all $\langle u^{(0)}, v^{(0)} \rangle$ with $\|u^{(0)}\| \leq 1$, $\|v^{(0)}\| \leq 1$, we have that $a = 1$, so $\|u^{(0)}\|_2 = 1$.

The above is typical of applications with subsidiary conditions in that extra structure must be taken into account. Sometimes the extra structure is not present. For example, if one tries to minimize $\mathscr{E}(\rho)$, given by (S.14), with the condition $\int \rho(x)\, dx = \lambda$, then a minimum exists if and only if $\lambda \leq \sum_{i=1}^{k} z_i$ (see the reference in the Notes).

Example 5 (existence of geodesics) Let M be a closed subset of $\mathbb{R}^\nu$, for example, a smoothly embedded surface. A continuous curve $\gamma\colon [0, 1] \to M \subset \mathbb{R}^\nu$ is called **rectifiable** if and only if its distributional derivative (thinking of γ as a function on $[0, 1]$ with values in $\mathbb{R}^\nu$), $\nabla\gamma$, lies in $L^1([0, 1], \mathbb{R}^\nu)$. For any rectifiable curve, one defines its length $L(\gamma)$ by

$$L(\gamma) = \int_0^1 |\nabla\gamma(s)|\, ds$$

We want to prove:

Theorem S.8 Let M be a closed subset of $\mathbb{R}^\nu$ and let x and y be in M. Suppose that there is a rectifiable curve lying in M with $\gamma(0) = x$, $\gamma(1) = y$. Then there is a curve $\tilde{\gamma}$ with these properties so that

$$L(\tilde{\gamma}) = d_{x,y} \equiv \inf\{L(\gamma) | \gamma \text{ lies in } M,\ \gamma(0) = x,\ \gamma(1) = y\}.$$

Such a minimizing curve is called **geodesic**.

Proof One cannot try to use Theorem S.6 directly on $L(\gamma)$ because L^1 is not reflexive. In fact, there is good reason why one cannot do this. For consider a reparametrization. Let f be a positive L^1 function on $[0, 1]$ with $\int_0^1 f(s)\,ds = 1$. Define

$$\tau(s) = \int_0^s f(t)\,dt$$

$$\tilde{\gamma}(s) = \gamma(\tau(s))$$

Then $\nabla\tilde{\gamma} = [(\nabla\gamma) \circ \tau]f$. Thus

$$L(\tilde{\gamma}) = \int_0^1 |\nabla\tilde{\gamma}|\,ds = \int_0^1 |(\nabla\gamma) \circ \tau|\,d\tau = L(\gamma)$$

Of course, this invariance of length is what makes length such a natural object. But it means the following: Let γ_n be a sequence of curves with $L(\gamma_n) \to d_{x,y}$. Let $\tilde{\gamma}_n$ be a curve which is a reparametrization of γ_n with the property that $\int_0^{1/n} |\nabla\tilde{\gamma}_n|\,ds = \frac{1}{2}$ (this can be done with a piecewise linear reparametrization). Then $L(\tilde{\gamma}_n)$ also converges to $d_{x,y}$, but $\tilde{\gamma}_n$ cannot have a reasonable limit. This says that one cannot hope to deal directly with $L(\gamma)$ by just being clever in the choice of space.

The way around this difficulty is what mathematicians often call "Dirichlet's principle" and what a physicist would describe by saying that "a free particle on a curved surface moves along geodesics at constant velocity." We define

$$E(\gamma) = \int_0^1 |\nabla\gamma(s)|^2\,ds$$

We shall use Theorem S.6 to find a curve γ_0 that minimizes E and then verify that $L(\gamma_0) \leq L(\gamma)$ for any γ (i.e., γ_0 is a geodesic). Along the way we shall show that $|\nabla\gamma_0(s)|$ is a constant (constant speed).

We begin by setting

$$Y \equiv \left\{ f \in L^2([0, 1]; \mathbb{R}^\nu, dx) \,\middle|\, x + \int_0^s f(t)\,dt \equiv \gamma^{(f)}(s) \in M \right.$$

$$\left. \text{for all } s \in [0, 1], \text{ and } \gamma^{(f)}(1) = y \right\}$$

and

$$\tilde{E}(f) \equiv \int_0^1 |f(s)|^2\,ds = E(\gamma^{(f)})$$

Clearly $\tilde{E}(f)$ is weakly lower semicontinuous and for any a, $\{f \mid \tilde{E}(f) \leq a\}$ is bounded. We defer the proof that it is nonempty for some a. Notice that

$$f \mapsto \int_0^s f(t)\, dt$$

is a continuous linear functional on $L^2([0, 1]; \mathbb{R}^\nu, dx)$ so, since M is closed, we have that Y is weakly closed. Hence there exists a γ_0 minimizing E.

Given any rectifiable curve γ define a function T by

$$T(s) \equiv L(\gamma)^{-1} \int_0^s |\nabla\gamma(t)|\, dt$$

We claim there is a continuous curve γ^* so that

$$\gamma^*(T(s)) = \gamma(s)$$

To see this, note that $T(s_0) = T(s_1)$ if and only if γ is constant on $[s_0, s_1]$. γ^* is called the **geodesic reparametrization** of γ, although in the special case that $|\nabla\gamma| = 0$ on an interval, it is not a reparametrization! However,

$$L(\gamma^*) = L(\gamma)$$

since γ is always a reparametrization of γ^*. Next notice that

$$|\nabla\gamma^*(s)| = L(\gamma)$$

since $\int_0^{T(s)} |\nabla\gamma^*(t)|\, dt = T(s)L(\gamma)$ for any $T(s)$. In particular, $E(\gamma^*) < \infty$, so that if there are rectifiable curves, there are also curves of finite energy. This shows that the set Y above is nonempty.

Next notice that by the Schwarz inequality, for any γ,

$$E(\gamma) \geq L(\gamma)^2 = L(\gamma^*)^2 = E(\gamma^*)$$

with equality only if $\gamma = \gamma^*$! Thus, the curve of minimum energy has $|\nabla\gamma_0| =$ constant. Moreover, for any other γ,

$$L(\gamma) = E(\gamma^*)^{\frac{1}{2}} \geq E(\gamma_0)^{\frac{1}{2}} = L(\gamma_0)$$

so γ_0 is indeed a geodesic. ∎

Supplement to V.5 Proofs of some theorems in nonlinear functional analysis

In this supplement we shall sketch the proof of the Leray–Schauder–Tychonoff theorem in the case where C has a separable topology, and we shall

state and prove the implicit function theorem. The Leray–Schauder–Tychonoff theorem is already highly nontrivial in the finite-dimensional case. We use some machinery which we take from algebraic topology. We state the following Theorem without proof:

Theorem S.9 For $n = 0, 1, 2, \ldots$, there is a map H_n from the set of topological spaces $\mathscr{T}$ to the set of abelian groups $\mathscr{A}$ so that for each $X \in \mathscr{T}$, $Y \in \mathscr{T}$ and continuous function $f: X \to Y$, there is a group homomorphism f_* from $H_n(X)$ to $H_n(Y)$ satisfying:

(i) If $f: X \to Y$ and $g: Y \to Z$, then $(g \circ f)_* = g_* \circ f_*$.

(ii) If $id: X \to X$ is the identity map on X, then $(id)_*$ is the identity map on $H_n(X)$.

(iii) If D^m is the m-dimensional disk, $\{x \in \mathbb{R}^m \mid |x| \leq 1\}$, and S^{m-1} is its boundary, then for $m \geq 2$, $H_{m-1}(D^m) = \{0\}$, the group consisting of a single element, and $H_{m-1}(S^{m-1}) = \mathbb{Z}$, the integers. For $n = 1$, $H_0(D^1) = \mathbb{Z}$ and $H_0(S^0) = \mathbb{Z} \oplus \mathbb{Z}$.

$H_n(X)$ is called the nth **homology group of** X. It is a measure of the number and type of $(n+1)$-dimensional "holes" in X.

Theorem S.10 (Brouwer fixed point theorem) Let C be a compact convex subset of $\mathbb{R}^n$ and suppose that $f: C \to C$ is continuous. Then f has a fixed point.

Proof Suppose first that $C = D^n$, the n-disk, and suppose that f has no fixed point. Given $x \in C$, let $g(x)$ be the point at which the line from $f(x)$ to x intersects S^{n-1}; i.e., $g(x)$ is determined by the conditions $g(x) = f(x) + \alpha(x - f(x))$ for some $\alpha > 0$, and $|g(x)| = 1$. Since $f(x)$ is assumed to be always distinct from x, it is easy to see that $x \to g(x)$ is a continuous map of D^n into S^{n-1}, and it is clear that this map leaves points in S^{n-1} fixed. Let h be the natural map of S^{n-1} into D^n obtained by inclusion. Then $g \circ h = id$. Thus, by parts (i) and (ii) of Theorem S.9, $g_* \circ h_* = id_*$ on homology. But for $n > 1$, $h_*: \mathbb{Z} \to \{0\}$ and $g_*: \{0\} \to \mathbb{Z}$ so that $g_* \circ h_*$ could not possibly be the identity on $\mathbb{Z}$. For $n = 1$, $h_*: \mathbb{Z} \oplus \mathbb{Z} \to \mathbb{Z}$ and $g_*: \mathbb{Z} \to \mathbb{Z} \oplus \mathbb{Z}$ so again $g_* \circ h_*$ cannot be the identity. Thus, we have a contradiction and conclude that f must have a fixed point if $C = D^n$.

Given a compact, convex $C \subset \mathbb{R}^n$, we can find a plane P of minimal dimension m and a vector v_0 so that $C \subset v_0 + P$. It is not hard to prove (Problem 20) that if we think of C as a topological subspace of $v_0 + P$, it has an interior point x_0. Thus, for any $v \in P$, $|v| = 1$, the set $\{t \geq 0 \mid x_0 + tv \in C\}$ is a non-

empty closed interval $[0, h(v)]$ since C is convex and closed. Further, $h(v) > 0$ since x_0 is an interior point of C in $v_0 + P$. h is a continuous map of the unit sphere S^{m-1} to $\mathbb{R}_+$ and the map

$$F: y \to [h((y - x_0)/|y - x_0|)]^{-1}(y - x_0)$$

is a homeomorphism of C onto D^m. Thus, the theorem for disks implies the general finite-dimensional case since all compact convex sets are homeomorphic to disks. ∎

Proof of Theorem V.19 (in the case where C has a countable base) Let $\{x_n\}$ be the countable dense set that we are assuming exists. For each n and m, we can find by the Hahn–Banach theorem an $\ell_{nm} \in X^*$ so that $\ell_{nm}(x_n) \neq \ell_{nm}(x_m)$. Since each ℓ_{nm} is bounded on C we can normalize the ℓ_{nm} so that $\sup_{y \in C} |\ell_{nm}(y)| \leq 2^{-n-m}$. Introduce a metric d on C by

$$d(x, y) = \left[\sum_{n,m} |\ell_{nm}(x - y)|^2\right]^{\frac{1}{2}}$$

Since d separates the x_n from one another, it is easy to see that it separates points. Moreover, d is continuous. Thus, the identity map from C with its original topology to C with the metric topology is a continuous bijection from a compact space to a Hausdorff space, and hence a homeomorphism.

By the definition of d, it is easy to see that it obeys the parallelogram law since this law is obeyed by each $|\ell_{nm}(x - y)|$ term separately. By mimicking the proof of the lemma to Theorem II.3, one sees that for each compact convex subset D of C and each $x \in C$ there is a unique point $\pi_D(x)$ in D closest to C and that π_D is continuous.

Now, given $\varepsilon > 0$, we can find, by compactness, a finite subset $y_1, \ldots, y_N$ of C so that any point in C lies within ε of some y_i. Let D be the set of points

$$\left\{\theta_1 y_1 + \cdots + \theta_n y_n | 0 \leq \theta_i \leq 1; \sum_{i=1}^{n} \theta_i = 1\right\}$$

D is a compact convex subset of C homeomorphic to a convex subset of some $\mathbb{R}^m$ ($m \leq n$). Moreover,

$$d(\pi_D(x), x) \leq \varepsilon \tag{S.19}$$

for all $x \in C$. Let $g: D \to D$ by $g(y) = \pi_D(f(y))$. By Theorem S.10, g has a fixed point x_ε. By (S.19), $d(f(x_\varepsilon), x_\varepsilon) \leq \varepsilon$. If x_0 is a limit point of the sequence $x_{1/n}$, then $d(f(x_0), x_0) = 0$, i.e., x_0 is a fixed point of f. ∎

* * *

To illustrate the uses of the contraction mapping theorem, we shall prove the implicit function theorem in Banach spaces. First, we define:

Definition Let X and Y be Banach spaces. We say that a function f from a neighborhood N_0 of x_0 in X to Y is differentiable at x_0 if and only if there exists a linear map $T \in \mathscr{L}(X, Y)$ so that

$$\lim_{x \to 0} \|x\|^{-1}[f(x_0 + x) - f(x_0) - Tx] = 0$$

We write $T \equiv (Df)(x_0)$. If N is open, if f is differentiable at all points in N, and if $x \to (Df)(x)$ is a norm continuous map of N into $\mathscr{L}(X, Y)$, we say that f is C^1 on N.

Theorem S.11 (implicit function theorem) Let X and Y be Banach spaces and let M_0 and N_0 be neighborhoods of $x_0 \in X$ and $y_0 \in Y$, respectively. Let $F: M_0 \times N_0 \to Y$ be a C^1 function. From the definitions it follows that for each $\langle x_1, y_1 \rangle \in M_0 \times N_0$, there are bounded operators $D_1 \in \mathscr{L}(X, Y)$ and $D_2 \in \mathscr{L}(Y, Y)$ so that $DF(x_1, y_1)$ is the linear operator given by $\langle x, y \rangle \to D_1 x + D_2 y$. At the point $\langle x_1, y_1 \rangle = \langle x_0, y_0 \rangle$, we set $T = D_1$, $S = D_2$.

Suppose that $F(x_0, y_0) = 0$ and that S has a bounded inverse. Then, there are neighborhoods $M_1 \subset M_0$ and $N_1 \subset N_0$ of x_0 and y_0 and a C^1 map $g: M_1 \to N_1$ so that $F(x, g(x)) = 0$ for all $x \in M_1$ and for each $x \in M_1$, $g(x)$ is the unique point y in N_1 satisfying $F(x, y) = 0$.

Proof We shall prove the existence and uniqueness of g. The verification that g is C^1 is left to the reader (Problem 21). First, choose ε_1 and δ so that

$$M_2 = \{x \mid \|x - x_0\| < \varepsilon_1\} \subset M_0, \qquad N_1 = \{y \mid \|y - y_0\| < \delta\} \subset N_0$$

and, for $\langle x, y \rangle \in M_2 \times N_1$,

$$\|I - S^{-1}D_2\| < \tfrac{1}{2}$$

Such a choice is possible since $S^{-1}D_2$ is norm continuous as $\langle x, y \rangle$ varies and equals I at $\langle x_0, y_0 \rangle$. Now, set

$$\alpha = \sup_{\langle x, y \rangle \in M_2 \times N_1} \|S^{-1}D_1\|$$

and let $M_1 = \{x \mid \|x - x_0\| < \varepsilon_2\}$ where ε_2 is chosen so that $\varepsilon_2 < \varepsilon_1$ and $\alpha\varepsilon_2 < \frac{1}{4}\delta$. We claim that for any fixed $x_1 \in M_1$, there exists exactly one $y \in N_1$ with $F(x_1, y) = 0$. By the fundamental theorem of calculus, for any C^1 function G,

$$\|G(a, b) - G(a', b')\| \leq c_1\|a - a'\| + c_2\|b - b'\| \qquad \text{(S.20)}$$

where

$$c_1 = \sup_{0 \le \theta \le 1} \|D_1 G(\theta a + (1-\theta)a', b')\|$$

and

$$c_2 = \sup_{0 \le \theta \le 1} \|D_2 G(a, \theta b + (1-\theta)b')\|$$

Given $x_1 \in M_1$ as above, let

$$H(y) \equiv y - S^{-1}F(x_1, y)$$

Using (S.20), we see that

$$\|H(y_0) - y_0\| \le \alpha \|x_1 - x_0\| < \tfrac{1}{4}\delta$$

Moreover, by (S.20) again,

$$\|H(y) - H(y')\| \le \tfrac{1}{2}\|y - y'\|$$

if y and y' are in N_1. Thus, H maps N_1 into itself and is a contraction. Notice that if N_1' is the open ball about y_0 of radius $\delta' < \delta$ where $|\delta' - \delta|$ is small, then this same argument shows that H takes N_1' into itself. Thus H has a unique fixed point y_1 in $\bar{N}_1' \subset N_1$. Since $H(y_1) = y_1$, we have $F(x_1, y_1) = 0$. ∎

Corollary 1 (inverse function theorem) Let Y be a Banach space and suppose that $f: N \to Y$ is a C^1 mapping where N is a neighborhood of $y_0 \in Y$. If $(Df)(y_0)$ is invertible, then there are neighborhoods N_1 of $f(y_0)$ and N_2 of y_0 and a C^1 map $g: N_1 \to N_2$ so that $f \circ g = I$ and $g(y)$ is the only point in N_2 with $f(g(y)) = y$.

Proof Let $F: N \times N \to Y$ by $F(x, y) = x - f(y)$. Then $D_2 F = -Df$ is invertible at $\langle f(y_0), y_0 \rangle$. Now apply the implicit function theorem. ∎

Corollary 2 (implicit function theorem—extended form) Let X, Y, and Z be Banach spaces and let N_0 and M_0 be neighborhoods of $x_0 \in X$ and $y_0 \in Y$, respectively. Let $F: M_0 \times N_0 \to Z$ be a C^1 function. Thus if $T \equiv (Df)(x_0, y_0)$, there are $R \in \mathscr{L}(X, Z)$ and $S \in \mathscr{L}(Y, Z)$ so that $T\langle x, y \rangle = Rx + Sy$. Suppose that $F(x_0, y_0) = 0$.

Suppose that S is onto Z and that there is a closed subspace $Y_1 \subset Y$ so that $Y_1 + \operatorname{Ker} S = Y$, $Y_1 \cap \operatorname{Ker} S = \{0\}$. Then, there is a neighborhood M_1 of x_0 and a C^1 function $g: M_1 \to Y$ with $g(x_0) = y_0$ so that $F(x, g(x)) = 0$ for all $x \in M_1$.

Proof Pick ε so that $\{y \mid \|y - y_0\| \leq \varepsilon\} \subset N_0$ and let G be the mapping of $M_0 \times \{y \in Y_1 \mid \|y\| < \varepsilon\}$ into Z given by $G(x, y) = F(x, y_0 + y)$. Then $D_2 G|_{\langle x_0, 0\rangle} = S \restriction Y_1$. By construction, $S \restriction Y_1$ is one to one, onto, and continuous. Thus Y_1 is isomorphic to Z and $S \restriction Y_1$ is invertible. By the basic implicit function theorem applied to G, g exists. ∎

Notice that the $g(x)$ in this last corollary need not be unique; it is unique if one adds the condition $g(x) - y_0 \in Y_1$. Two cases where a suitable Y_1 exists whenever S is onto are the case dim $Y < \infty$ and the case where Y is a Hilbert space.

Supplement to VI.5 Applications of compact operators

In Section VI.4 we outlined the application of compact operators to the solution of the Dirichlet problem for bounded regions in $\mathbb{R}^2$. In this supplement we give two simpler applications. Consider the following initial-boundary value problem in partial differential equations (q is continuous):

$$\begin{aligned} u_t(x, t) - u_{xx}(x, t) + q(x)u(x, t) &= 0, \qquad 0 \leq x \leq 1 \\ u(x, 0) &= f(x) \\ u(0, t) &= 0 = u(1, t) \end{aligned} \tag{S.21}$$

There are various physical situations that are modeled by this equation. For example, $u(x, t)$ could be the density at x at time t of a gas in a pipe of length one. If $q(x)$ is zero, then we have the usual diffusion equation with diffusion constant one. If $q(x)$ is positive, then $q(x)u(x, t)$ units of gas per unit length per unit time are removed at $\langle x, t\rangle$ by a chemical reaction with other material in the pipe. It is reasonable that the amount removed at $\langle x, t\rangle$ be dependent on the local density $u(x, t)$ and on the position in the pipe through $q(x)$. The condition $u(x, 0) = f(x)$ gives the gas density at $t = 0$, and the boundary conditions reflect a situation where the gas can freely escape at the ends so that the density at the ends is effectively zero.

Following the method of eigenfunction expansions, one first tries to find solutions of the differential equation and boundary conditions of the form $\psi(t)\varphi(x)$. Plugging into the differential equation, we find that

$$\frac{\psi'(t)}{\psi(t)} = \frac{\varphi''(x)}{\varphi(x)} - q(x)$$

for all x and t, so both sides equal a constant, call it $-\lambda$. Thus, we must solve the differential equation

$$\psi'(t) + \lambda\psi(t) = 0$$

and the eigenvalue problem

$$-\varphi''(x) + q(x)\varphi(x) - \lambda\varphi(x) = 0 \tag{S.22}$$
$$\varphi(0) = 0 = \varphi(1)$$

Recall what happens in the case $q(x) \equiv 0$. In that case we can solve the differential equation explicitly, and we find that the eigenvalue problem has a solution if and only if $\lambda = \lambda_n \equiv (n\pi)^2$, $n = 1, 2, \ldots$, in which case

$$\varphi(x) = \varphi_n(x) \equiv \sqrt{2}\sin n\pi x \qquad \text{and} \qquad \psi(t) = \psi_n(t) \equiv e^{-(n\pi)^2 t}$$

Thus, for each n, $\psi_n(t)\varphi_n(x)$ solves the differential equation and boundary conditions in (S.21). Since the differential equation is linear and the boundary conditions are homogeneous, any linear combination of these solutions is again a solution of the differential equation and the boundary conditions. So, one tries to write the solution of (S.21) in the form

$$u(x, t) = \sum_{n=1}^{\infty} a_n \varphi_n(x)\psi_n(t)$$

and tries to choose the coefficients $\{a_n\}$ so that

$$f(x) = u(x, 0) = \sum_{n=1}^{\infty} a_n \varphi_n(x) \tag{S.23}$$

The fact that one can do this is just the classical fact that every (sufficiently nice) function $f(x)$ can be represented by a convergent Fourier (sine) series.

Now, consider the case where $q(x)$ is not identically zero. At first sight the problem seems almost impossible. It is not immediately evident that the eigenvalue problem will have solutions for a discrete set of λ_n. Even if it did, we would not expect to be able to compute the λ_n or the corresponding eigenfunctions φ_n explicitly. And, even if we could compute the φ_n explicitly, how could we expect them to obey the many identities for sine and cosine which are used in proving the classical Fourier series theorem? Notice, however, that if the eigenvalue problem (S.22) does have solutions λ_n, φ_n, then

$$\int_0^1 \varphi_n(x)\varphi_m(x)\,dx = 0$$

if $n \neq m$ and $\lambda_n \neq \lambda_m$. This can easily be checked (Problem 22) by substituting using the differential equation, and integrating by parts. Thus, the eigenfunctions, if they exist, are orthogonal in the sense of (real) $L^2[0, 1]$. This suggests that we reformulate our problem as a Hilbert space problem. What we are really asking is whether (S.22) has a set of solutions $\{\varphi_n(x)\}$, with corresponding eigenvalues λ_n, which are an orthonormal basis for $L^2[0, 1]$. If this is true, then every $f \in L^2[0, 1]$ can be written in the form (S.22). Further, the $\varphi_n(x)$ are automatically twice continuously differentiable. Also, one can show by integration by parts (Problem 22) that any λ_n that do exist must satisfy $\lambda_n \geq \inf q(x)$. In the proof below it turns out that the λ_n can have no finite limit point, so only finitely many of them can be nonpositive. Therefore the series

$$u(x, t) = \sum_{n=1}^{\infty} a_n e^{-\lambda_n t} \varphi_n(x)$$

will converge very rapidly for $t > 0$, so that one can check that $u(x, t)$ satisfies the differential equation (S.21) for $t > 0$. $u(x, t)$ satisfies the boundary conditions since the $\varphi_n(x)$ do, and u satisfies the initial condition in the sense that

$$\|u(x, t) - f(x)\|_2 \to 0$$

as $t \downarrow 0$. Thus, we can solve our original problem in partial differential equations if we show that (S.22) has a family of solutions $\{\varphi_n\}$ which are a basis for $L^2[0, 1]$.

For simplicity, we shall assume that $q(x)$ is continuous and that $q(x) \geq 0$. The positivity hypotheses is easily removed (see Problem 22). Let $u_0(x)$ be a nonzero solution of $-u''(x) + q(x)u(x) = 0$ that satisfies $u_0(0) = 0$ and let $u_1(x)$ be a nonzero solution that satisfies $u_1(1) = 0$. The Wronskian of the two solutions $W = u_0'(x)u_1(x) - u_0(x)u_1'(x)$ is constant on $[0, 1]$ and equals zero if and only if $u_0(x) = \alpha u_1(x)$ for some α. But if this is so, $u_0(0) = 0 = u_0(1)$ so

$$\int_0^1 (u_0')^2 \, dx = -\int_0^1 u_0'' u_0 \, dx = -\int_0^1 q(x) u_0^2 \, dx$$

which implies that $u_0'(x) \equiv 0$ so $u_0(x)$ is constant. But since $u_0(0) = 0$, we would have $u_0(x) \equiv 0$. This contradiction shows that $W \neq 0$. Thus, for $y \in [0, 1]$, we can define

$$k(x, y) = \begin{cases} u_0(x)u_1(y)W^{-1}, & x \leq y \\ u_0(y)u_1(x)W^{-1}, & x > y \end{cases}$$

and set

$$(T\psi)(x) = \int_0^1 k(x, y)\psi(y) \, dy$$

Then, by Theorem VI.23, T is a Hilbert–Schmidt (and therefore compact) operator on $L^2[0, 1]$. We shall show that T is a right inverse to $L = -d^2/dx^2 + q(x)$. Suppose that $\psi(x) \in L^2[0, 1]$ and write

$$(T\psi)(x) = W^{-1}u_1(x)\int_0^x u_0(y)\psi(y)\,dy + W^{-1}u_0(x)\int_x^1 u_1(y)\psi(y)\,dy$$

Since $\psi \in L^2$, the indefinite integrals are absolutely continuous and

$$\frac{d}{dx}(T\psi)(x) = W^{-1}u_1'(x)\int_0^x u_0(y)\psi(y)\,dy + W^{-1}u_0'(x)\int_x^1 u_1(y)\psi(y)\,dy$$

Again we see that $(d/dx)(T\psi)(x)$ is absolutely continuous and

$$\begin{aligned}\frac{d^2}{dx^2}(T\psi)(x) &= W^{-1}u_1''(x)\int_0^x u_0(y)\psi(y)\,dy + W^{-1}u_0''(x)\int_x^1 u_1(y)\psi(y)\,dy \\ &\quad + W^{-1}u_1'(x)u_0(x)\psi(x) - W^{-1}u_0'(x)u_1(x)\psi(x) \\ &= q(x)\int_0^1 k(x, y)\psi(y)\,dy - \psi(x)\end{aligned}$$

Thus, $(T\psi)(x)$ is twice differentiable, with second derivative in $L^2[0, 1]$ and

$$-\frac{d^2}{dx^2}(T\psi)(x) + q(x)(T\psi)(x) = \psi(x)$$

that is, $LT\psi = \psi$. Notice also that, because $u_0(0) = 0 = u_1(1)$, $T\psi$ satisfies $(T\psi)(0) = 0 = (T\psi)(1)$. In the terminology of Chapter VIII, we would say that T takes $L^2[0, 1]$ into the domain of $-(d^2/dx^2) + q(x)$.

As pointed out above, T is compact and since $k(x, y) = k(y, x)$, T is self-adjoint. Thus by the Hilbert–Schmidt theorem (Theorem VI.16), there is an orthonormal basis $\{\varphi_n\}$ and a sequence of numbers $\{\mu_n\}$ so that

$$T\varphi_n = \mu_n\varphi_n$$

$LT = I$, so we have

$$\varphi_n = LT\varphi_n = \mu_n L\varphi_n$$

which shows that $\mu_n \neq 0$ and

$$-\varphi_n''(x) + q(x)\varphi_n(x) = \frac{1}{\mu_n}\varphi_n$$

and, since φ_n is in the range of T, we automatically have

$$\varphi_n(0) = 0 = \varphi_n(1)$$

Notice that $\mu_n \to 0$ since T is compact. Thus the λ_n cannot have any finite limit point. Since they are bounded below (Problem 22), we have $\lambda_n \to \infty$. We summarize:

Theorem S.12 Suppose that $q(x)$ is a continuous function on $[0, 1]$. Then there exists an orthonormal basis $\{\varphi_n\}$ for $L^2[0, 1]$ consisting of twice continuously differentiable functions and a sequence of numbers $\lambda_n \to \infty$ such that

$$-\varphi_n''(x) + q(x)\varphi_n(x) = \lambda_n \varphi_n(x)$$

In Problem 23 some of these ideas are extended to space dimension three. The unbounded operator L discussed above has a compact resolvent at $\lambda = 0$ and therefore, by the first resolvent formula, L has a compact resolvent for all $\lambda \in \rho(L)$. Operators with compact resolvent are discussed in Section XIII.14.

As a second application of compact operators we prove the following classical theorem of Weyl:

Theorem S.13 Suppose that A and B are self-adjoint operators on a Hilbert space such that $A - B$ is compact. Then $\sigma_{ess}(A) = \sigma_{ess}(B)$.

Proof $\sigma_{ess}(\cdot)$ is defined in Section VII.3 and according to Weyl's criterion (Theorem VII.12), $\lambda \in \sigma_{ess}(A)$ if and only if there is an orthonormal sequence $\{\psi_n\}$ such that $\|(A - \lambda)\psi_n\| \to 0$. Suppose that this is the case. Since the ψ_n are orthonormal, they converge weakly to zero. By Theorem VI.11, this implies that $\|(A - B)\psi_n\| \to 0$ since $A - B$ is compact. Thus,

$$\|(B - \lambda)\psi_n\| \leq \|(A - \lambda)\psi_n\| + \|(A - B)\psi_n\| \to 0$$

Therefore, by Weyl's criterion, $\lambda \in \sigma_{ess}(B)$. This shows that $\sigma_{ess}(A) \subset \sigma_{ess}(B)$. By symmetry, $\sigma_{ess}(B) \subset \sigma_{ess}(A)$. ∎

Various generalizations of this theorem as well as applications are discussed in Section XIII.4.

Supplement to VIII.7 Monotone convergence for forms

In this supplement we prove some very useful approximation theorems for positive self-adjoint operators.

Definition Let t and s be two positive quadratic forms on a Hilbert space $\mathscr{H}$. We say that $t \leq s$ if and only if $Q(t) \supset Q(s)$ and $t(\varphi, \varphi) \leq s(\varphi, \varphi)$ for all $\varphi \in Q(s)$.

Note that this definition says that if t is an extension of s to a larger domain, then $t \leq s$. In particular, $\bar{t} \leq t$ for any closable form t.

Theorem S.14 Let $t_1, t_2, \ldots, t_n, \ldots$ be a sequence of closed, positive quadratic forms satisfying $0 \leq t_1 \leq \cdots \leq t_n \leq \cdots$. Suppose that

$$Q(t_\infty) = \left\{ \varphi \in \mathscr{H} \,\middle|\, \sup_n t_n(\varphi, \varphi) < \infty \right\}$$

is dense. Then the quadratic form

$$t_\infty(\varphi, \varphi) = \lim_{n \to \infty} t_n(\varphi, \varphi) = \sup_n t_n(\varphi, \varphi)$$

with domain $Q(t_\infty)$ is closed. Moreover, if T_n, T_∞ are the operators corresponding to these forms, then $T_n \to T_\infty$ in strong resolvent sense.

We give two proofs of this theorem below. Note that by the Schwarz inequality applied to $t_n(\varphi, \varphi)$, $Q(t_\infty)$ is a vector space and that, by polarization, the values of $t_\infty(\varphi, \varphi)$ determine those of $t_\infty(\varphi, \psi)$.

To state the second convergence theorem, we need some preliminaries. We say that a form t is **closable** if and only if it has a closed extension. Then there always exists a smallest closed extension which we call $\bar{t}$, that is, a closed extension whose domain is contained in the domains of all other closed extensions.

Theorem S.15 Let t be any positive quadratic form. Then, there exists a largest closable quadratic form t_r that is smaller than t.

We can now state:

Theorem S.16 Let $t_1, \ldots, t_n, \ldots$ be a sequence of closed, positive, quadratic forms with $t_1 \geq t_2 \geq \cdots \geq 0$. Let $Q(t_\infty) = \bigcup_n Q(t_n)$ and

$$t_\infty(\varphi, \varphi) = \lim_n t_n(\varphi, \varphi) = \inf_n t_n(\varphi, \varphi)$$

Let T_n be the operator corresponding to t_n and let S correspond to the closure of $(t_\infty)_r$. Then $T_n \to S$ in strong resolvent sense.

Notice that part of the first convergence theorem has no analog in the second.

Example Let $Q = \{f \in \mathscr{H} = L^2(-\infty, \infty) \mid f' \in L^2(-\infty, \infty)\}$. It can be shown (see Example 3 in Section X.2) that any $f \in Q$ is continuous and that the t_n defined on Q by

$$t_n(f, g) = n^{-1} \int_{-\infty}^{\infty} \overline{f'(x)} g'(x)\, dx + \overline{f(0)} g(0)$$

are closed, positive, quadratic forms. Clearly $t_1 \geq t_2 \geq \cdots$ and $t_\infty(f, g) = \overline{f(0)} g(0)$. But t_∞ is *not* closed or even closable. In fact $(t_\infty)_r = 0$ so $S = 0$ in this case.

The following result, which is of independent interest, is relevant to the monotone convergence theorems.

Theorem S.17 Let S and T be two positive self-adjoint operators and let s, t be the corresponding quadratic forms. Then $s \leq t$ if and only if $(T + 1)^{-1} \leq (S + 1)^{-1}$.

Proof Suppose that $s \leq t$. Then for any φ, $(T + 1)^{-1}\varphi \in D(T) \subset Q(t) \subset Q(s)$, so

$$\begin{aligned}
(\varphi, (T + 1)^{-1}\varphi) &= ((S + 1)^{-\frac{1}{2}}\varphi, (S + 1)^{\frac{1}{2}}(T + 1)^{-1}\varphi) \\
&\leq (\varphi, (S + 1)^{-1}\varphi)^{\frac{1}{2}}((T + 1)^{-1}\varphi, (S + 1)(T + 1)^{-1}\varphi)^{\frac{1}{2}} \\
&\leq (\varphi, (S + 1)^{-1}\varphi)^{\frac{1}{2}}((T + 1)^{-1}\varphi, (T + 1)(T + 1)^{-1}\varphi)^{\frac{1}{2}} \\
&\leq (\varphi, (S + 1)^{-1}\varphi)^{\frac{1}{2}}(\varphi, (T + 1)^{-1}\varphi)^{\frac{1}{2}}
\end{aligned}$$

proving that $(T + 1)^{-1} \leq (S + 1)^{-1}$. The first inequality is just the Schwarz inequality and the second uses $s \leq t$.

Conversely, suppose that $(T + 1)^{-1} \leq (S + 1)^{-1}$. Let $\eta \in Q(s)$. Then

$$\begin{aligned}
\|(T + 1)^{-\frac{1}{2}}(S + 1)^{\frac{1}{2}}\eta\|^2 &= ((S + 1)^{\frac{1}{2}}\eta, (T + 1)^{-1}(S + 1)^{\frac{1}{2}}\eta) \\
&\leq ((S + 1)^{\frac{1}{2}}\eta, (S + 1)^{-1}(S + 1)^{\frac{1}{2}}\eta) \\
&= (\eta, \eta)
\end{aligned}$$

Thus $(T + 1)^{-\frac{1}{2}}(S + 1)^{\frac{1}{2}}$ is a bounded map of norm at most one from $Q(s)$ to $\mathscr{H}$. It follows that its adjoint is everywhere defined and has norm at most one, i.e., $\mathrm{Ran}((T + 1)^{-\frac{1}{2}}) = Q(t) \subset Q(s)$ and for any $\eta = (T + 1)^{-\frac{1}{2}}\varphi \in Q(t)$,

$$(s + 1)(\eta, \eta) = \|(S + 1)^{\frac{1}{2}}(T + 1)^{-\frac{1}{2}}\varphi\|^2 \leq \|\varphi\|^2 = (t + 1)(\eta, \eta) \quad \blacksquare$$

Our first proof of Theorem S.14 depends on the notion of lower semicontinuous function defined in the supplement to Section IV.5.

Theorem S.18 Let t be a positive quadratic form. Define $\tilde{t}(\varphi)$ on $\mathscr{H}$ by

$$\tilde{t}(\varphi) = \begin{cases} t(\varphi, \varphi) & \text{if } \varphi \in Q(t) \\ \infty & \text{if } \varphi \notin Q(t) \end{cases}$$

Then t is closed if and only if $\tilde{t}$ is lower semicontinuous.

Proof Given any positive quadratic form t, we can define $\mathscr{H}_{+1,t}$ to be the *completion* of $Q(t)$ in the norm $[t(\varphi, \varphi) + (\varphi, \varphi)]^{\frac{1}{2}}$. The bounded linear map $\varphi \mapsto \varphi$ of $Q(t)$ into $\mathscr{H}$ extends to a map i of $\mathscr{H}_{+1,t}$ into $\mathscr{H}$. It is not hard to see (Problem 24 and Section X.3) that t is closable if and only if i is one to one, and in that case $\bar{t}$ has domain Ran i with $\bar{t}(\varphi, \psi) = (i^{-1}(\varphi), i^{-1}(\psi))_{+1} - (\varphi, \psi)$.

If t is not closable, we can find $\varphi \in \mathscr{H}_{+,1}$ with $i(\varphi) = 0$, i.e., φ_n in $Q(t)$ so that $\varphi_n \to 0$ and $t(\varphi_n - \varphi_m, \varphi_n - \varphi_m) \to 0$ but with $\lim_n t(\varphi_n, \varphi_n)$ nonzero, say 2. We can pass to a subsequence with $t(\varphi_n - \varphi_m, \varphi_n - \varphi_m) \leq \frac{1}{2}$ and $t(\varphi_n, \varphi_n) \geq 1$. Let $\eta_n = \varphi_1 - \varphi_n$. Then $\eta_n \to \varphi_1$ but $\tilde{t}(\varphi_1) \geq 1 > \frac{1}{2} \geq \underline{\lim}\, \tilde{t}(\eta_n)$ so $\tilde{t}$ is not lower semicontinuous.

Suppose next that t is closable but not closed. Then, we can find $\varphi \notin Q(t)$, $\varphi_n \in Q(t)$ with $\varphi_n \to \varphi$ and $t(\varphi_n - \varphi_m, \varphi_n - \varphi_m) \to 0$. Then $\tilde{t}(\varphi_n)$ is Cauchy, and so it has a finite limit α; thus $\tilde{t}(\varphi) = \infty > \alpha = \underline{\lim}\, \tilde{t}(\varphi_n)$. Again, $\tilde{t}$ is not lower semicontinuous.

Thus, we see that if $\tilde{t}$ is lower semicontinuous, then t is closed. Conversely, suppose that t is closed. Let T denote the corresponding self-adjoint operator. Let $T_n = TP_n$ where P_n is the spectral projection of T for the interval $[0, n)$. Let $\varphi_m \to \varphi$ and fix n. Noticing that $T_n \leq T$ and $T_n^{\frac{1}{2}}\varphi_m \to T_n^{\frac{1}{2}}\varphi$ since T_n is bounded, we have that

$$(\varphi, T_n\varphi) = \lim_m (\varphi_m, T_n\varphi_m) \leq \underline{\lim}(\varphi_m, T\varphi_m)$$

Since $\tilde{t}(\varphi) = \lim_n (\varphi, T_n\varphi)$ by the monotone convergence theorem for the spectral measure $d\mu_\varphi$, we have that

$$\tilde{t}(\varphi) \leq \underline{\lim}\, \tilde{t}(\varphi_m)$$

i.e., $\tilde{t}$ is lower semicontinuous. ∎

First Proof of Theorem S.14 By definition $\tilde{t}_\infty(\varphi) = \sup_n \tilde{t}_n(\varphi)$ for any φ where $\tilde{s}$ is defined in Theorem S.18. By that theorem, each $\tilde{t}_n$ is lower semicontinuous. Thus, if $\varphi_m \to \varphi$, then

$$\tilde{t}_n(\varphi) \leq \underline{\lim}\, \tilde{t}_n(\varphi_m) \leq \underline{\lim}\, \tilde{t}_\infty(\varphi_m)$$

since $\tilde{t}_n \leq \tilde{t}_\infty$. Taking the sup over n, we see that $\tilde{t}_\infty$ is lower semicontinuous and thus t_∞ is closed.

Now let T_∞ be the operator corresponding to t_∞. By Theorem S.15, $(\varphi, (T_n + 1)^{-1}\varphi) \geq (\varphi, (T_\infty + 1)^{-1}\varphi)$ and $(\varphi, (T_n + 1)^{-1}\varphi)$ is monotone decreasing. It follows that

$$\lim_n (\varphi, (T_n + 1)^{-1}\varphi) = \inf_n (\varphi, (T_n + 1)^{-1}\varphi)$$

has a nonzero value, so we can find a self-adjoint A with zero kernel so that $(T_n + 1)^{-1} \to A$ weakly. Let s be the quadratic form of $S \equiv A^{-1} - 1$. Since $(T_n + 1)^{-1} \geq A \geq (T_\infty + 1)^{-1}$, we have $t_n \leq s \leq t_\infty$. Since $\tilde{t}_\infty = \sup_n \tilde{t}_n$, we have that $\tilde{s} = \tilde{t}_\infty$, i.e., $A = (T_\infty + 1)^{-1}$. Thus $(T_n + 1)^{-1}$ converges weakly to $(T_\infty + 1)^{-1}$. By a similar argument this holds if 1 is replaced by any $c \geq 0$; and then by analyticity we have weak convergence of the resolvents on $\mathbb{C}\backslash[0, \infty)$. As noted in Section VIII.7, this implies strong resolvent convergence. ∎

Proof of Theorem S.15 Let $\mathscr{H}_{+1}$ and i be as defined in the proof of Theorem S.18. Let P be the projection (orthogonal in the natural inner product on $\mathscr{H}_{+1}$) onto Ker i and let $Q = 1 - P$. For $\varphi \in Q(t)$, let $j(\varphi)$ be its natural image in $\mathscr{H}_{+1}$, so that $i \circ j = 1$ and $(j(\varphi), j(\varphi))_{+1} = t(\varphi, \varphi) + (\varphi, \varphi)$. Define

$$t_r(\varphi, \psi) = (Qj(\varphi), j(\psi))_{+1} - (\varphi, \psi)$$

$$t_s(\varphi, \psi) = (Pj(\varphi), j(\psi))$$

We claim that t_r is closable; indeed, the $\mathscr{H}_{+1}$ associated to t_r is just Ran Q and the corresponding $\tilde{i}$ is just the above i restricted to Ran Q. Since Ran $Q \cap$ Ran $P = \{0\}$, this $\tilde{i}$ is one to one.

Next, we note that $t_r \geq 0$. For $iQ = i(1 - P) = i$ since Ran $P \subset$ Ker i. Thus, for any $\varphi \in Q(t)$,

$$\begin{aligned}(\varphi, \varphi) &= (i \circ j(\varphi), i \circ j(\varphi)) \\ &= (iQj(\varphi), iQj(\varphi)) \\ &\leq (Qj(\varphi), Qj(\varphi))_{+1}\end{aligned}$$

since i is norm decreasing from $\mathscr{H}_{+1}$ to $\mathscr{H}$.

Now suppose that h is a positive closable form and $h \leq t$. By the corollary to Theorem II.4, there exists a unique positive operator A on $\mathscr{H}_{+1}$ with $(h + 1)(\varphi, \psi) = (j(\varphi), Aj(\psi))_{+1}$. Let $\varphi \in$ Ran $P \subset \mathscr{H}_{+1}$. Pick $\eta_n \in Q(t)$ with $j(\eta_n) \equiv \varphi_n \to \varphi$. Then $i(\varphi_n) = \eta_n \to i(\varphi) = 0$. Moreover, since the φ_n are Cauchy in $\mathscr{H}_{+1}$, they will be Cauchy in the h norm. Since h is closable, $h(\varphi_n, \varphi_n) \to 0$, i.e., $(\varphi, A\varphi) = 0$. It follows that $h(\varphi, \varphi) = h(Q\varphi, Q\varphi) \leq (Q\varphi, Q\varphi)_{+1}$, so that $h \leq t_r$. Thus t_r is the largest closable form less than t. ∎

Second Proof of Theorem S.14 We give a second proof only of the fact that t_∞ is closed. The rest of the proof is identical to the first proof.

Clearly $t_n \leq t_\infty$; and since t_n is closable, we have that $t_n \leq (t_\infty)_r$. But then $\sup_n t_n(\varphi, \varphi) \leq (t_\infty)_r(\varphi, \varphi)$, i.e., $t_\infty = (t_\infty)_r$, so t_∞ is closable and therefore $\bar{t}_\infty \leq t_\infty$. Moreover, given $\psi_m \in Q(t_\infty)$, such that $\psi_m \to \psi$ in the t_∞ norm, we have that $\psi_m \to \psi$ in t_n norm, so $t_n(\psi, \psi) \leq \bar{t}_\infty(\psi, \psi)$, i.e., $t_n \leq \bar{t}_\infty$. Thus, as above $t_\infty = \bar{t}_\infty$. ∎

Proof of Theorem S.16 As in the proof of Theorem S.14, T_n converges in strong resolvent sense to an operator S given by

$$(\varphi, (S + 1)^{-1}\varphi) = \sup_n (\varphi, (T_n + 1)^{-1}\varphi)$$

Let s be the quadratic form of S. By Theorem S.17, $s \leq t_n$ so $s \leq t_\infty$. Since $s = s_r$, $s \leq (t_\infty)_r$ and thus, as in the last proof, $s \leq \overline{(t_\infty)_r}$. On the other hand, if T_∞ corresponds to $\overline{(t_\infty)_r}$, then, since $\overline{(t_\infty)_r} \leq t_\infty \leq t_n$, we have that $(T_\infty + 1)^{-1} \geq (T_n + 1)^{-1}$. Taking limits in n, $(T_\infty + 1)^{-1} \geq (S + 1)^{-1}$ so $s \geq \overline{(t_\infty)_r}$, i.e. $s = \overline{(t_\infty)_r}$. ∎

Supplement to VIII.8 More on the Trotter product formula

In this section we want to consider positive self-adjoint operators A and B and prove that

$$\text{s-lim}_{n\to\infty}(e^{-tA/n}e^{-tB/n})^n = e^{-tC} \tag{S.24}$$

for suitable C under various hypotheses. As we explain in the Notes, some of the ideas below can be used to prove the Trotter product formula for general contraction semigroups on Banach spaces including Theorem VIII.30.

Theorem S.19 (Chernoff's theorem; self-adjoint case) Let A be a positive self-adjoint operator and let $f(t)$ be a family of self-adjoint operators with $0 \leq f(t) \leq 1$. Define $S(t) = t^{-1}(1 - f(t))$. If $S(t)$ converges in strong resolvent sense to A as $t \downarrow 0$, then for any fixed t,

$$s\text{-}\lim_{n\to\infty} f\left(\frac{t}{n}\right)^n = e^{-tA} \tag{S.25}$$

Proof By hypothesis and Theorem VIII.20,

$$\operatorname*{s-lim}_{n\to\infty} \exp\left(-tS\left(\frac{t}{n}\right)\right) = e^{-tA}$$

so we need only show that

$$\operatorname*{s-lim}_{n\to\infty}\left[\exp\left(-tS\left(\frac{t}{n}\right)\right) - f\left(\frac{t}{n}\right)^n\right] \equiv \operatorname*{s-lim}_{n\to\infty} Q(n,t) = 0 \tag{S.26}$$

But, since $tS(t/n) = n(1 - f(t/n))$ obeys $0 \le tS(t/n) \le n$, we have that

$$Q(n,t) = G_n\left(tS\left(\frac{t}{n}\right)\right)$$

where

$$G_n(x) = \begin{cases} e^{-x} - \left(1 - \dfrac{x}{n}\right)^n, & 0 \le x \le n \\ e^{-x}, & x \ge n \end{cases}$$

Thus (S.26) follows if we show that $\lim_n \|G_n\|_\infty = 0$. This is easily established by using the fact that $G_n(x) \to 0$ pointwise, and therefore, since

$$|G_n'(x)| = \left|e^{-x} - \left(1 - \frac{x}{n}\right)^{n-1}\right| \le 1$$

it goes to zero uniformly on bounded intervals. Moreover,

$$\sup_{n\ge x}\left(1 - \frac{x}{n}\right)^n \le \sup_{a\ge 1}\left[\left(1 - \frac{1}{a}\right)^a\right]^x \le e^{-x}$$

since $u(x) = (1 - x^{-1})^x$ obeys

$$(\ln u)'(x) = \sum_{k=1}^{\infty} \frac{1}{x^k}\left(1 - \frac{1}{k}\right) > 0$$

on $(1, \infty)$ and $\lim_{x\to\infty} u(x) = e^{-1}$. ∎

It is now easy to prove the last half of Theorem VIII.31.

Theorem S.20 (Trotter product formula, self-adjoint case) Let A and B be positive self-adjoint operators such that $A + B$ is essentially self-adjoint on $D(A) \cap D(B)$. Then (S.24) holds where C is the closure of $A + B$.

Proof Let $f(t) = e^{-tA/2}e^{-tB}e^{-tA/2}$ and suppose that $\eta \in D(A) \cap D(B)$. Then,

$$t^{-1}(1 - f(t))\eta = e^{-tA/2}e^{-tB}[t^{-1}(1 - e^{-tA/2})\eta] + e^{-tA/2}[t^{-1}(1 - e^{-tB})\eta] + t^{-1}(1 - e^{-tA/2})\eta$$

Using the fact that the product of uniformly bounded, strongly convergent sequences of operators is strongly convergent,

$$t^{-1}(1 - f(t))\eta \to (A + B)\eta = C\eta$$

for $\eta \in D(A) \cap D(B)$. By Theorem VIII.25a, $t^{-1}(1 - f(t))$ converges to C in strong resolvent sense so, by Theorem S.19, s-lim $f(t/n)^n = e^{-tC}$.

Since s-lim$_{t\to 0} f(t) = I$, we have that $f(t/n)^n - f(t/n)^{n-1} = f(t/n)^{n-1} \times (f(t/n) - 1)$ converges strongly to zero. But

$$(e^{-tA/n}e^{-tB/n})^n = e^{-tA/2n}f(t/n)^{n-1}e^{-tA/2n}e^{-tB/n}$$

so (S.24) holds since products of uniformly bounded convergent sequences are convergent. ∎

Theorem S.20 can be strengthened:

Theorem S.21 (Kato's strong Trotter product formula) Let A and B be positive self-adjoint operators with $Q(A) \cap Q(B)$ dense. Then the quadratic form $\langle \varphi, \psi \rangle \to (\varphi, A\psi) + (\varphi, B\psi)$ with domain $Q(A) \cap Q(B)$ is closed. Let C be the corresponding self-adjoint operator. Then (S.24) holds.

Proof That the given form is closed is easy and left to the problems (Problem 25). By the same argument as at the end of the last proof, it suffices to show that s-lim $f(t/n)^n = e^{-tC}$ where

$$f(t) = e^{-tA/2}e^{-tB}e^{-tA/2}$$

By Chernoff's theorem, we need only show that

$$S(t) \equiv t^{-1}(1 - f(t))$$

converges to C in strong resolvent sense. Define

$$A(t) = t^{-1}(1 - e^{-At}), \qquad B(t) = t^{-1}(1 - e^{-Bt})$$

and $C(t) = A(\tfrac{1}{2}t) + B(t)$. Notice that

$$\|tA(t)\| \leq 1; \qquad \|tB(t)\| \leq 1 \tag{S.27}$$

$$\text{s-lim}_{t\downarrow 0}\, tA(t) = \text{s-lim}_{t\downarrow 0}\, tB(t) = 0 \tag{S.28}$$

Moreover, since $t^{-1}(1 - e^{-xt}) = x\int_0^1 e^{-xts}\,ds$ is positive and monotone decreasing in t for x fixed, we see that $A(t)$ and $B(t)$ are monotone increasing to A and B, respectively, as $t \downarrow 0$. It follows from the first monotone convergence theorem for forms (Theorem S.14) that for $b > 0$,

$$(b + C(t))^{-1} - (b + C)^{-1} \overset{s}{\to} 0 \tag{S.29}$$

Rewriting $S(t)$ in terms of $A(t)$ and $B(t)$, we see that

$$S(t) = C(t) + E(t)$$

where

$$E(t) = \frac{t}{4} A\left(\frac{t}{2}\right)(1 - tB(t))A\left(\frac{t}{2}\right) - \frac{t}{2} A\left(\frac{t}{2}\right)B(t) - \frac{t}{2} B(t)A\left(\frac{t}{2}\right)$$

Fix $b > 0$ and let

$$Q(t) = (C(t) + b)^{-\frac{1}{2}}E(t)(C(t) + b)^{-\frac{1}{2}}$$

We claim that

$$(\varphi, Q(t)\varphi) \geq -\frac{\sqrt{2}}{2}\|\varphi\|^2 \tag{S.30}$$

and

$$\underset{t\downarrow 0}{\text{s-lim}}\, Q(t) = 0 \tag{S.31}$$

Accepting (S.30) and (S.31) for the moment, we can complete the proof. Since all operators involved are bounded, we have that

$$(S(t) + b)^{-1} = (C(t) + b)^{-\frac{1}{2}}(1 + Q(t))^{-1}(C(t) + b)^{-\frac{1}{2}}$$

Thus,

$$(S(t) + b)^{-1} - (C(t) + b)^{-1} = -(C(t) + b)^{-\frac{1}{2}}(1 + Q(t))^{-1}Q(t)(C(t) + b)^{-\frac{1}{2}}$$

By (S.30), $\|(1 + Q(t))^{-1}\| \leq 2/(2 - \sqrt{2})$ so since $\|(C(t) + b)^{-\frac{1}{2}}\| \leq b^{-\frac{1}{2}}$, we need only that $\text{s-lim}_{t\downarrow 0} Q(t)(C(t) + b)^{-\frac{1}{2}} = 0$. This follows from (S.29) and (S.31). Thus

$$\underset{t\downarrow 0}{\text{s-lim}}[(S(t) + b)^{-1} - (C(t) + b)^{-1}] = 0$$

so, by (S.29), $S(t)$ converges to C in strong resolvent sense.

Therefore, we need only prove (S.30) and (S.31). We begin by noting that the first term of $E(t)$ is positive, so

$$\begin{aligned}(\varphi, Q(t)\varphi) &\geq -\mathrm{Re}\left((C(t)+b)^{-\frac{1}{4}}\varphi,\, tA\left(\frac{t}{2}\right)B(t)(C(t)+b)^{-\frac{1}{4}}\varphi\right)\\ &\geq -\|t^{\frac{1}{4}}B(t)^{\frac{1}{4}}\|\left\|t^{\frac{1}{4}}A\left(\frac{t}{2}\right)^{\frac{1}{4}}\right\|\left\|A\left(\frac{t}{2}\right)^{\frac{1}{4}}(C(t)+b)^{-\frac{1}{4}}\varphi\right\|\\ &\quad\times\|B(t)^{\frac{1}{4}}(C(t)+b)^{-\frac{1}{4}}\varphi\|\\ &\geq -\frac{\sqrt{2}}{2}\left((C(t)+b)^{-\frac{1}{4}}\varphi,\left[A\left(\frac{t}{2}\right)+B(t)\right](C(t)+b)^{-\frac{1}{4}}\varphi\right)\\ &\geq -\frac{\sqrt{2}}{2}(\varphi,\varphi)\end{aligned}$$

where in the last step we used $\|C(t)(C(t)+b)^{-1}\| \leq 1$, and in the step before that the inequality $xy \leq \frac{1}{2}(x^2+y^2)$. This proves (S.30).

To prove (S.31), first note that

$$\left\|A\left(\frac{t}{2}\right)^{\frac{1}{4}}(C(t)+b)^{-\frac{1}{4}}\varphi\right\|^2 + \|B(t)^{\frac{1}{4}}(C(t)+b)^{-\frac{1}{4}}\varphi\|^2 + b\|(C(t)+b)^{-\frac{1}{4}}\varphi\|^2 = \|\varphi\|^2 \tag{S.32}$$

(S.32) implies in the first place that

$$\left\|A\left(\frac{t}{2}\right)^{\frac{1}{4}}(C(t)+b)^{-\frac{1}{4}}\right\| \leq 1 \qquad \|B(t)(C(t)+b)^{-\frac{1}{4}}\| \leq 1 \tag{S.33}$$

Moreover, the analog of (S.32) for A, B, C replacing $A(\frac{1}{2}t)$, $B(t)$, $C(t)$, shows that weak convergence of the three operators in (S.32) as $t \downarrow 0$ implies strong convergence (Problem 26). Because of (S.33), one only needs

$$(\varphi, B(t)^{\frac{1}{4}}(C(t)+b)^{-\frac{1}{4}}\psi) \to (\varphi, B^{\frac{1}{4}}(C+b)^{-\frac{1}{4}}\psi)$$

for φ in a dense set. This convergence for φ in $D(B)$ and any ψ follows from (S.29). Thus

$$\operatorname*{s-lim}_{t\downarrow 0} B(t)^{\frac{1}{4}}(C(t)+b)^{-\frac{1}{4}} = B^{\frac{1}{4}}(C+b)^{-\frac{1}{4}}$$

and similarly for $A(\frac{1}{2}t)$ and A. Now, to prove (S.31), take a typical term in the sum like

$$(C(t)+b)^{-\frac{1}{4}}\frac{t}{4}A\left(\frac{t}{2}\right)(1-tB(t))A\left(\frac{t}{2}\right)(C(t)+b)^{-\frac{1}{4}}$$

and write it as $\alpha\beta\gamma\delta\varepsilon$ with

$$\alpha = (C(t) + b)^{-\frac{1}{4}} A\left(\frac{t}{2}\right)^{\frac{1}{4}}$$

$$\beta = \frac{1}{4}\left[tA\left(\frac{t}{2}\right)\right]^{\frac{1}{4}}$$

$$\gamma = (1 - tB(t))$$

$$\delta = \left[tA\left(\frac{t}{2}\right)\right]^{\frac{1}{4}}$$

and

$$\varepsilon = A(t)^{\frac{1}{4}}(C(t) + b)^{-\frac{1}{4}}$$

α, β, γ, δ, and ε are uniformly bounded and since ε is strongly convergent, and $\delta \to 0$ strongly as $t \to 0$, the product converges strongly to zero. ∎

Additional supplement Uses of the maximum principle

It is not evident from looking at the basic definitions in functional analysis that the theory of analytic functions should play any role in the subject at all. That complex variable techniques *are* applicable is due mainly to the analyticity of the resolvent (Theorem VI.5) and to the analyticity properties of the Fourier transforms of functions with restricted support (see Section IX.3). Since analytic functions have such strong properties, it is not surprising that theorems from complex analysis are useful, indeed central, when many of the basic objects under study have analyticity properties. One of the most useful of these theorems is the maximum principle which states: Let f be an analytic function on an open bounded subset D of $\mathbb{C}$ and suppose that f *is* continuous on $\bar{D}$. Then $|f|$ achieves its maximum on the boundary. Often, it is not the maximum principle itself which is applied, but a corollary of it or an extended maximum principle for an unbounded domain. See, for example, the three line lemma (in the Appendix to Section IX.4), Theorem XI.89, Theorem XII.18, the lemma to Corollary 4 in Section XIII.4 (this is equivalent to Example 2 below via a conformal mapping), Carlson's theorem (the lemma to Theorem XIII.61), and the Borel–Carathéodory theorem (Lemma 5 in Section XIII.17).

In this section we want to acquaint the reader with a nice trick which is the main device for proving many of the extended maximum principles and corollaries of the maximum principle. Here is the idea: Let f be analytic in D and continuous on $\bar{D}$. If h is another analytic function in D which is continuous on $\bar{D}$ and which satisfies $h(z_0) = 1$ for some $z_0 \in D$, then

$$|f(z_0)| = |h(z_0)f(z_0)| \leq \sup_{w \in \partial D} |h(w)|\,|f(w)|$$

By choosing h cleverly one can arrange to give more weight to some parts of the boundary where we have more information. We can let h depend on z_0 and often it depends on an auxiliary parameter. We illustrate this idea by two examples.

Example 1 Let $f(z)$ be a function which is continuous in the region $R = \{z | 0 \leq \operatorname{Re} z \leq 1,\ \operatorname{Im} z \geq 0\}$, analytic in the interior. Suppose that $\sup_{z \in R} |f(z)| < \infty$ and that $\lim_{y \to \infty} |f(iy)| = 0$. Then, for each $\varepsilon > 0$,

$$\lim_{y \to \infty} \sup_{0 \leq x \leq 1 - \varepsilon} |f(x + iy)| = 0 \tag{S.34}$$

To prove this, let $C \equiv \sup_{z \in R} |f(z)|$ and let $z_0 = x_0 + iy_0$ be a point in R. Let the region $D(y_0)$ be given by

$$D(y_0) = \{z \in R | 0 < \operatorname{Re} z < 1,\ \tfrac{1}{2}y_0 < \operatorname{Im} z < \tfrac{3}{2}y_0\}$$

and take

$$h(z) = e^{(z - z_0)^2 - B(z - z_0)}$$

where B is a positive constant to be chosen in a moment. Since h is analytic and $h(z_0) = 1$, the maximum principle for D implies that

$$|f(z_0)| \leq \max\{a_1, a_2, a_3, a_4\}$$

where

$$a_1 = \max_{\frac{1}{2}y_0 \leq y \leq \frac{3}{2}y_0} |f(1 + iy)h(1 + iy)| \leq Ce^{-B(1 - x_0) + 1}$$

$$a_2 = \max_{0 \leq x \leq 1} |f(x + \tfrac{1}{2}iy_0)h(x + \tfrac{1}{2}iy_0)| \leq Ce^{B - (y_0^2/4) + 1}$$

$$a_3 = \max_{0 \leq x \leq 1} |f(x + \tfrac{3}{2}iy_0)h(x + \tfrac{3}{2}iy_0)| \leq Ce^{B - (y_0^2/4) + 1}$$

$$a_4 = \max_{\frac{1}{2}y_0 \leq y \leq \frac{3}{2}y_0} |f(iy)h(iy)| \leq Ce^{B+1} \max_{y \geq \frac{1}{2}y_0} |f(iy)|$$

We now choose B (depending on y_0) so that

$$e^{-2B} = e^{-y_0^2/4} + \max_{y \geq \frac{1}{2}y_0} |f(iy)|$$

This implies that $B < y_0^2/8$, so $a_2(y_0) \to 0$ and $a_3(y_0) \to 0$ as $y_0 \to \infty$. Also, $B(y_0) \to \infty$ as $y_0 \to \infty$, so $a_4(y_0) \to 0$ since $e^B \max_{y \geq \frac{1}{2}y_0} |f(iy)| = e^{-B} - e^{B-(y_0^2/4)}$. Finally, $a_1(y_0) \to 0$ as $y_0 \to \infty$ uniformly for all $x_0 \leq 1 - \varepsilon$, so (S.34) holds.

Example 2 Let $\{f_n(z)\}_{n=1}^{\infty}$ be a sequence of functions which are analytic in the unit disc $R = \{z \mid |z| < 1\}$ and which satisfy $\sup_{n, |z|<1} |f_n(z)| \equiv C < \infty$. Fix some $\theta_0 > 0$ and suppose that for each n, f_n can be extended to be continuous on

$$R \cup \{z \mid |z| = 1, |\arg z| \leq \theta_0\}, \text{ and that } \lim_{n \to \infty} \sup_{|\theta| \leq \theta_0} |f_n(e^{i\theta})| = 0$$

We shall show that for each $\delta > 0$,

$$\lim_{n \to \infty} \sup_{|z| \leq 1-\delta} |f_n(z)| = 0 \tag{S.35}$$

Let $D_{\theta_0} = \{z \in R \mid |\arg z| < \theta_0\}$ and define $g_n(z) = f_n(z^{2\theta_0/\pi})$ for $z \in D_{\pi/2} \cup \{z \mid |z| = 1, |\arg z| \leq \pi/2\}$. Then $\sup_{n, z \in D_{\pi/2}} |g_n(z)| \leq C$ and

$$\lim_{n \to \infty} \sup_{|\theta| \leq \pi/2} |g_n(e^{i\theta})| = 0$$

On the straight piece of the boundary of $D_{\pi/2}$ we have no information except boundedness of the boundary values of g_n. Take $z \in D_{\pi/2}$ and set $h(z) = e^{B(z-z_0)}$ for $B > 0$ fixed. Then, by the maximum principle for $D_{\pi/2}$,

$$\begin{aligned} |g_n(z_0)| &\leq \sup_{z \in \partial D_{\pi/2}} |e^{B(z-z_0)} g_n(z)| \\ &\leq C_1(B) \sup_{|\theta| \leq (\pi/2)} |g_n(e^{i\theta})| + Ce^{-Bx_0} \end{aligned}$$

Thus, $\lim_{n \to \infty} |g_n(z_0)| \leq Ce^{-Bx_0}$ and since B is arbitrary, we conclude that $\lim_{n \to \infty} |g_n(z_0)| = 0$. Thus, $\lim_{n \to \infty} |f_n(z_0)| = 0$ for $z_0 \in D_{\theta_0}$. Standard methods in complex function theory now permit one to show easily that $f_n(z) \to 0$ uniformly on compact subsets of D_{θ_0} and analytic continuation then allows one to conclude (S.35). The reader is asked to provide these details in Problem 28.

We remark that in functional analysis the maximum principle and its extensions are typically applied to Banach space-valued analytic functions. This generalization causes no problems as the reader is asked to show in Problem 29. In Problem 30, the reader can use the technique of this section to prove a maximum principle for an unbounded domain.

NOTES

Supplement II.2 Theorem S.1 and its proof by these means is due to J. von Neumann, "On Rings of Operators, III," *Ann. Math.* **41** (1940), 127. The Bergmann kernel is named after the work of S. Bergman, "Ueber Hermitische unendliche Formen, die zu einem Bereich gehören, nebst Anwendungen auf Fragen der Abbildung durch Funktionen zweier komplexen Veränderlichen," *Math. Z.* **29** (1929), 640–677. For further discussion and applications to partial differential equations and several complex variables, see S. Bergman, *The Kernel Function and Conformal Mapping*, Amer. Math. Soc. Survey, No. 5 (2nd ed., 1970), Amer. Math. Soc., Providence, Rhode Island.

Supplement IV.5 Theorem S.6 is a basic technique in nonlinear functional analysis sometimes called the *direct method of the calculus of variations*. It is a descendent of ideas of Hilbert. The existence properties of the Thomas–Fermi equations are discussed in E. Lieb and B. Simon, "The Thomas–Fermi Theory of Atoms, Molecules and Solids," *Advances in Mathematics* **23** (1977), 22–116, and of the Hartree equation in E. Lieb and B. Simon, "The Hartree–Fock Theory for Coulomb Systems," *Commun. Math. Phys.* **53** (1977), 185–194.

For further discussion and examples of this method, see Chapter 6 of M. Berger, *Nonlinearity and Functional Analysis*, Academic Press, New York, 1977.

There is a readable discussion of the existence of geodesics which does not use Theorem S.6 but which uses instead ideas from differential geometry in M. Spivak, *A Comprehensive Introduction to Differential Geometry*, Vol. I, Publish or Perish, Cambridge, Massachusetts, 1970. Theorem S.8 is closely related to what is usually called the Hopf–Rinow theorem.

Our proof of the existence of geodesics actually shows that there is a minimizing path in each homotopy class (see Problem 18). For a beautiful application of this result to prove the existence of periodic orbits in certain classical mechanical systems, see p. 248 of V. I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer-Verlag, New York, 1978.

Supplement V.5 For a discussion of homology and the Brouwer fixed point theorem, see any book on algebraic topology, e.g., the book of Hilton and Wylie quoted in the notes to Section V.5 or J. Vick, *Homology Theory*, Academic Press, New York, 1973. There is an "elementary" proof of the Brouwer theorem in J. Milnor, "Analytic proofs of the 'hairy ball theorem' and the Brouwer fixed point theorem," *Amer. Math. Mon.* **85** (1978), 521–524, with more details in J. Franklin, *Methods of Mathematical Economics*, Springer, New York, 1980.

Supplement VIII.7 Versions of the monotone convergence theorems that suppose that t_∞ is closed go back at least as far as Kato's book quoted in the Notes to Section VIII.6. That t_∞ is automatically closed in the increasing case is due to D. Robinson, *The Thermodynamic Pressure in Quantum Statistical Mechanics*, Springer Lecture Notes in Physics **9** (1971), Springer-Verlag, New York, where an essentially equivalent result appears. Unaware of this work, E. B. Davies found Theorem S.18 and the resulting proof of Theorem S.14 which we give as the first proof in "A Model for Absorbtion or Decay," *Helv. Phys. Acta* **48** (1975), 365–382, as did T. Kato (quoted in the next mentioned paper). See also B. Simon, "Lower Semicontinuity of Positive Quadratic Forms," *Proc. Roy. Soc. Edinburgh* **29** (1977), 267–273.

The decomposition Theorem S.15 and the identification of the limit in Theorem S.16 are due to B. Simon, "A Canonical Decomposition for Quadratic Forms with Applications to Monotone Convergence Theorems," *J. Functional Anal.* **28** (1978), 377–385.

There is a version of the first monotone convergence theorem even in the case where $Q(t_\infty)$ is not dense; see Simon's two papers quoted on page 385.

Supplement VIII.8 Chernoff's theorem was proven in his *J. Functional Anal.* paper quoted in the Notes to Section VIII.8. He proves it when A is the generator of any contraction semigroup on any Banach space and $f(t)$ any family of contractions (operators with $\|f(t)\| \leq 1$). One advantage of the form of his theorem is that it implies that for many real-valued functions F and G,

$$\left[F\left(\frac{tA}{n}\right)G\left(\frac{tB}{n}\right)\right] \to e^{-t(A+B)}$$

e.g., under the hypotheses of Theorem S.20,

$$\left[\left(1+\frac{tA}{n}\right)^{-1}\left(1+\frac{tB}{n}\right)^{-1}\right]^n \to e^{-t(A+B)}$$

The proofs in this section are such that it is easy to verify the uniformity of convergence in the t variable as t runs through compact subsets of $[0,\infty)$.

Kato's strong version of the product formula is proven in T. Kato, "Trotter's Product Formula for an Arbitrary Pair of Self-Adjoint Contraction Semigroups," in *Topics in Functional Analysis* (G. C. Rota, ed.), Academic Press, New York, 1978, pp. 185–195. Extension to more than two factors and some nonlinear operators can be found in T. Kato and K. Masuda, "Trotter's Product Formula for Nonlinear Semigroups Generated by the Subdifferentials of Convex Functionals," *J. Math. Soc. Japan* **30** (1978), 169–178. Extensions to include generators of holomorphic semigroups can be found in Kato's paper and a *kind* of Trotter product formula for unitary groups under the hypotheses of Theorem S.21 is proven in T. Ichinose, "A Product Formula and Its Application to the Schrödinger Equation," to appear.

Kato actually proves a stronger result than we prove in Theorem S.21. Namely, he proves that whenever A and B are positive self-adjoint operators on a Hilbert space, then s-$\lim(e^{-A/n}e^{-B/n})^n = e^{-C}P$ where P is the projection onto $\overline{Q(A)\cap Q(B)}$ and C is the obvious operator on Ran P.

There has been a considerable amount of work on nonlinear product formulas. See, for example: H. Brezis and A. Pazy, "Semigroups of Nonlinear Contractions on Convex Sets," *J. Functional Anal.* **5** (1970), 237–281; H. Brezis and A. Pazy, "Convergence and Approximation of Semigroups of Nonlinear Operators in Banach Spaces," *J. Functional Anal.* **9** (1972), 63–74; Paul R. Chernoff, "Product Formulas, Nonlinear Semigroups, and Addition of Unbounded Operators," *Memoirs of the American Mathematical Society*, Number 140; A. J. Chorin, T. J. R. Hughes, M. F. McCracken, and J. E. Marsden, "Product Formulas and Numerical Algorithms," *Comm. Pure Appl. Math.* **XXXI** (1978), 205–256; M. G. Crandall and T. M. Liggett, "Generation of Semi-Groups of Nonlinear Transformations on General Banach Spaces," *Amer. J. Math.* **93** (1971), 265–298; J. Marsden, "On Product Formulas for Nonlinear Semigroups," *J. Functional Anal.* **13** (1973), 51–72; Eric Schechter, "Well-Behaved Evolutions and Trotter Products," Thesis, University of Chicago, 1978; G. F. Webb, "Exponential Representation of Solutions to an Abstract Semi-Linear Differential Equation," *Pacific J. Math.* **70** (1977), 269–279; and Fred B. Weissler, "Construction of Non-Linear Semi-Groups Using Product Formulas," *Israel J. Math.* **29** (1978), 265–275. These product formulas play an important role in the existence theorems for certain classes of nonlinear partial differential equations.

Additional Supplement The results of this section and Problem 25 are often called Phragmén-Lindelöf theorems. Some of the original papers are: J. Hadamard, "Sur les fonctions entières," *Bull. Soc. Math. France* **24** (1896), 186-187; E. Phragmén, "Sur une extension d'un théorème classique de la théorie des fonctions," *Acta Math.* **28** (1904), 351-368; E. Lindelöf and E. Phragmén, "Sur une extension d'un principe classique de l'analyse et sur quelque propriétés des fonctions monogènes dans le voisinage d'un point singulier," *Acta Math.* **31** (1908), 381-406; E. Lindelöf, "Sur un principe général d'analyse et ses applications à la theorie de la représentation conforme," *Acta Soc. Sci. Finn.* **46**(4) (1915), 1-35. For simple proofs see L. Ahlfors, "On Phragmén-Lindelöf's principle," *Trans. Amer. Math. Soc.* **41** (1937), 1-8.

PROBLEMS

1. Use Theorem S.1 to prove Theorems I.19 and I.20 in the general σ-finite case.

2. (a) Let $\Omega = \{z \mid |z| < 1\}$ and define $T_r: L^2(\Omega) \to L^2(\Omega)$ by

$$(T_r f)(z) = f(zr)$$

for $0 < r < 1$. Prove that $T_r f \to f$ as $r \to 1$ for any $f \in L^2$. (*Hint*: Prove it for $f \in C(\bar{\Omega})$ and use an $\varepsilon/3$ argument.)

(b) If f is analytic in $\{z \mid |z| < 1 + \varepsilon\}$ for some $\varepsilon > 0$, prove that the Taylor series for f about $z = 0$ converges to f in $L^2(\Omega)$.

(c) Conclude that $\{z^n\}_{n=0}^{\infty}$ is a basis for $\mathscr{A}(\Omega)$.

3. Let K be the Bergmann reproducing kernel for some set Ω.

(a) Prove that $|K(z, w)| \leq K(z, z)^{\frac{1}{2}} K(w, w)^{\frac{1}{2}}$.

(b) Prove that $K(z, z) + K(w, w) - K(z, w) - K(w, z) \geq 0$.

(c) Fix $z \in \Omega$. Let

$$a_{ij}(z) = \frac{\partial}{\partial x_i} \frac{\partial}{\partial y_j} K(x_1 + ix_2, y_1 + iy_2)\Big|_{x_1 + ix_2 = z = y_1 + iy_2}$$

Prove that $a = \{a_{ij}\}$ is a positive definite matrix.

Remark $\{a_{ij}(z)\}$ defines a metric in the sense of Riemann geometry and introduces a natural geometric structure into Ω. For example, if Ω is the unit disk, the resulting geometry is one of the standard non-Euclidean geometries.

4. (a) Prove that equality holds in (S.8) only if $a = b^{q-1}$.

(b) Suppose that $\|f\|_p = \|g\|_q = 1$. Prove that equality in (S.7) holds if and only if $|g| = |f(x)|^{p-1}$.

(c) Prove that equality holds in general in (S.7) only if g is zero (a.e.) or if

$$g(x) = \lambda \overline{f(x)} |f(x)|^{p-2}$$

for some fixed $\lambda \in \mathbb{C}$.

(d) Let $h \in L^1$. Prove that $\int h \, d\mu = \|h\|_1$ if and only if h is a.e. nonnegative.

(e) Prove that $|\int f(x) g(x) \, d\mu(x)| \leq \|f\|_p \|g\|_q$ with equality only if $g = |f|^{p-1} \operatorname{sgn} f$ where $\operatorname{sgn} f = \bar{f}/|f|$ at points where $f \neq 0$ and $\operatorname{sgn} f = 0$ otherwise.

5. Use the method of the proof of (S.8) to prove Young's inequality: $xy \le e^x + y \log y - y$ for all $x > 0$, $y > 0$.

†6. By mimicking the proof of Theorem IV.16 and its lemma, prove that any $L \in (L^p)^*$ is a finite linear combination of positive functionals.

†7. (a) Let X be σ-finite and let $Y \subset X$. Given $L \in L^p(X, d\mu)^*$, define $\tilde{L} \in L^p(Y, d\mu)^*$ by $\tilde{L}(f) = L(\tilde{f})$ where $\tilde{f}$ is the function on X obtained by extending f to be zero on $X \setminus Y$. Prove that $\|\tilde{L}\| \le \|L\|$.

(b) Given Theorem S.4 for finite measure spaces, prove the same result in the σ-finite case.

8. Prove that no sequence that is not eventually constant can be a universal net.

9. (a) Let α be a function of bounded variation on $[0, 1]$. Prove that for any $t \in [0, 1]$, $\alpha(t - 0) \equiv \lim_{s \uparrow t} \alpha(s)$ and $\alpha(t + 0) \equiv \lim_{s \downarrow t} \alpha(s)$ exist.

(b) Show that $\alpha(t - 0) = \alpha(t + 0)$ for all but at most countably many t's.

(c) Show that among all α's leading to the same Riemann–Stieltjes integral, there is precisely one with $\alpha(0) = 0$ and $\alpha(t) = \alpha(t - 0)$ for all t.

(d) Show that if $\tilde{\alpha}$ obeys $\tilde{\alpha}(0) = 0$, $d\tilde{\alpha} = d\alpha$ where α is the function of part (c), and Variation (α) = Variation$(\tilde{\alpha})$, then for any t, either

$$\alpha(t - 0) \le \tilde{\alpha}(t) \le \alpha(t + 0) \qquad \text{or} \qquad \alpha(t + 0) \le \tilde{\alpha}(t) \le \alpha(t - 0)$$

10. Let α be of bounded variation. Show that

(a) $(b - a)^{-1} \int_a^b (x - a)\, d\alpha = \alpha(b - 0) - [\int_a^b \alpha(x)\, dx](b - a)^{-1}$ and use Problem 9a to show that

$$\lim_{b \downarrow a} (b - a)^{-1} \int_a^b (x - a)\, d\alpha = 0$$

(b) Fix $a < c$ and for δ small let f_δ be given by

$$f_\delta(x) = \begin{cases} 0, & x \le a \quad \text{or} \quad x \ge c \\ \delta^{-1}(x - a), & a \le x \le a + \delta \\ 1, & a + \delta \le x \le c - \delta \\ \delta^{-1}(c - x), & c - \delta \le x < c \end{cases}$$

Show that

$$\lim_{\delta \downarrow 0} \int f_\delta(x)\, d\alpha(x) = \alpha(c - 0) - \alpha(a + 0)$$

(c) Prove that if $\int \cdot\, d\alpha$ is a positive Riemann–Stieltjes integral on $C[0, 1]$, then the α with $\alpha(t) = \alpha(t - 0)$ is monotone nondecreasing so that corresponding Lebesgue–Stieltjes measure is positive.

†11. Let $F: X \to (-\infty, \infty]$. Show that F is lower semicontinuous if and only if for all a, $\{x \mid F(x) \le a\}$ is closed.

†12. Let C be a convex subset of a locally convex space X. Use the separating hyperplane theorem (Theorem V.4) to show that C is closed in the topology of X if and only if C is closed in the weak $(\sigma(X, X^*))$ topology.

13. A function F on a vector space V is called *strictly convex* if and only if $F(\lambda x + (1-\lambda)y) < \lambda F(x) + (1-\lambda)F(y)$ for $x \neq y$ and $0 < \lambda < 1$. Show that a strictly convex function has at most one point where its minimum value is taken and that any stationary point of F is its minimizing point. Use these ideas to show that (S.12) has a unique L^2 solution.

14. Let $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ be consistent norms on a vector space V in the sense of Section IX.4. Let

$$\|x\|^+ = \inf\{\|y\|^{(0)} + \|z\|^{(1)} | x = y + z\}$$

Let X_0, X_1, X_+ be the completions of V in the norms $\|\cdot\|^{(0)}$, $\|\cdot\|^{(1)}$, $\|\cdot\|^+$. Let $\|\cdot\|_{(0)}$, $\|\cdot\|_{(1)}$ be the norm of X_0^*, X_1^*. Prove that $X_+^* = X_0^* \cap X_1^*$ with the norm

$$\|\ell\| = \max\{\|\ell\|_{(0)}, \|\ell\|_{(1)}\}$$

15. Let H be a C^1 convex function on $(-\infty, \infty)$ with $|H(u)| \leq C|u|^p$ for some $p \geq 1$. Let $f \in C_0^\infty$. Show that

$$-\Delta u + H'(u) = f$$

has a solution in $L^p \cap L^2$.

16. Let $h(x) = [\max\{1, |x|\}]^{-1}$ and $g(x) = |x|^{-1} - h(x)$. In the language of Example 3 of the supplement to Section IV.5, prove that $h \in K^*$ and that $g \in L^{\frac{4}{3}}$. Conclude that

$$f \to \int f(x)V(x)\,dx$$

is an element of $L^{\frac{4}{3}} + K^*$.

†17. Fill in the missing details of Examples 2 and 4 of the supplement to Section IV.5.

18. Let M be a closed subset of $\mathbb{R}^\nu$ and suppose that $\{\gamma \text{ in } M \mid \gamma(0) = x, \gamma(1) = y\}$ lies in several homotopy classes. Fix one such class c and let

$$Y_c = \{f \in Y \mid \gamma^{(f)} \in c\}$$

where Y and $\gamma^{(f)}$ are given in the proof of Theorem S.8. Show that Y_c is weakly closed and conclude that there is a curve in c minimizing the length among all curves in c.

19. Prove Theorem S.8 "directly" by showing that if γ_n is such that $L(\gamma_n) \to \inf\{L(\gamma)\}$ and that if γ_n is geodesically parametrized, then $\{\gamma_n\}$ is equicontinuous and so by the Ascoli–Arzela theorem, there exists a subsequence $\gamma_n \to \gamma_\infty$.

20. Let C be a compact convex subset of $\mathbb{R}^n$ so that $0 \in C$ and the vectors in C span $\mathbb{R}^n$. Prove that C has nonempty interior.

21. Verify that the map g in Theorem S.11 is C^1.

22. (a) Show that if $\lambda_n, \varphi_n(x)$ and $\lambda_m, \varphi_m(x)$ are solutions of (S.22) and $\lambda_n \neq \lambda_m$, then

$$\int_0^1 \varphi_n(x)\varphi_m(x)\,dx = 0$$

(b) Prove that any λ for which there is a $\varphi(x)$ satisfying (S.22) must satisfy

$$\lambda \geq \min_{0 \leq x \leq 1} q(x)$$

(c) Using part (b), extend the proof of Theorem S.12 to the case where $q(x)$ can be negative.

23. The purpose of this problem is to extend Theorem S.12 to three dimensions. Let $\Omega \subset \mathbf{R}^3$ be a bounded open region with smooth boundary $\partial\Omega$. Let $G_0(x, y) \equiv (4\pi|x - y|)^{-1}$.
   (a) Let $y \in \Omega$. We suppose that the Dirichlet problem is solvable (see Section VI.4) and let $H(x, y)$ be the solution of $-\Delta_x H(x, y) = 0$, $H(x, y) = G_0(x, y)$ for x on $\partial\Omega$. Let $G_D(x, y) = G_0(x, y) - H(x, y)$. Using the maximum principle, show that

$$0 \leq G_D(x, y) \leq G_0(x, y)$$

   (b) For $f \in C_0^\infty(\Omega)$ define $(T_0 f)(x) = \int_\Omega G_D(x, y) f(y)\, dy$. Prove that $(-\Delta)T_0 f = f = T_0(-\Delta)f$ and $(T_0 f)(x) = 0$ for x on $\partial\Omega$. Conclude that G_D is symmetric.
   (c) Prove that T_0 is Hilbert-Schmidt on $L^2(\Omega)$.
   (d) Show that any eigenvalue of T_0 is positive and, since T_0 is compact, conclude that T_0 is a positive operator.
   (e) Suppose that $q(z) > 0$ for all $z \in \Omega$ and that q is C^∞. Using the fact that T_0 is positive, prove that

$$f(x) = -\int_\Omega G_D(x, z) q(z) f(z)\, dz$$

   has no solutions. Conclude that there is a unique solution $k(x, y)$ of

$$k(x, y) = G_D(x, y) - \int_\Omega G_D(x, z) q(z) k(z, y)\, dz$$

   for all $y \in \Omega$.
   (f) Use the maximum principle to prove that $0 \leq k(x, y) \leq G_D(x, y)$ and conclude that $k(x, y)$ is the kernel of a Hilbert-Schmidt operator T.
   (g) Prove that T is a two-sided inverse for $-\Delta + q$ with the boundary condition $f \restriction \partial\Omega = 0$. Show that the eigenvalue problem

$$-\Delta u(x) + q(x)u(x) - \lambda u(x) = 0 \qquad \text{for} \quad x \in \Omega$$

$$u(x) = 0 \qquad \text{for} \quad x \in \partial\Omega$$

   has an L^2 basis of eigenfunctions.

24. Fill in the details of the $\mathscr{H}_{+1,l}$ construction of Theorem S.18.

†25. Let A and B be closed semibounded quadratic forms with $Q \equiv Q(A) \cap Q(B)$ dense. Prove that the form $\langle \varphi, \psi \rangle \to (\varphi, A\psi) + (\varphi, B\psi)$ on $Q \times Q$ defines a *closed* semibounded quadratic form.

†26. (a) Let $\varphi_n \to \varphi$ weakly and $\|\varphi_n\| \to \|\varphi\|$. Prove that $\varphi_n \to \varphi$ in norm (*Hint*: Compute $\|\varphi - \varphi_n\|^2$.)
   (b) Let $\varphi_n^{(1)} \to \varphi^{(1)}, \ldots, \varphi_n^{(j)} \to \varphi^{(j)}$ weakly and

$$\sum_{i=1}^{j} \|\varphi_n^{(i)}\|^2 \to \sum_{i=1}^{j} \|\varphi^{(i)}\|^2$$

   Prove that $\varphi_n^{(i)} \to \varphi^{(i)}$ in norm.

27. Let A and B be semibounded self-adjoint operators with $A + B$ essentially self-adjoint on $D(A) \cap D(B)$. Let C be the operator associated to the form of Problem 25. Prove that $C = \overline{A + B}$.

† 28. Complete the complex variables argument outlined at the end of Example 2 in the additional supplement.

29. Let X be a Banach space and let D be a bounded open subset of $\mathbb{C}$. Let $f: \bar{D} \to X$ in such a way that for each $\ell \in X^*$, $\ell \circ f$ is analytic in D and continuous on $\bar{D}$. Prove that

$$\sup_{z \in D} \|f(z)\| = \sup_{z \in \partial D} \|f(z)\|$$

30. Suppose that f is analytic in the wedge $N = \{z \mid |z| > 0, \alpha < \arg z < \beta\}$, where $\beta - \alpha < \pi$, and continuous on $\bar{N}$. Suppose further that $|f(z)| \leq C_1 e^{C_2|z|}$ for all $z \in N$ and some constants C_1, C_2. Prove that f obeys an extended maximum principle

$$|f(z)| \leq \max_{r} \{|f(re^{i\alpha})|, |f(re^{i\beta})|\}$$

(*Hint*: Consider the case $-\pi/2 < \alpha < \beta < \pi/2$ and let $h(z) = e^{-\mu z^{\mu}}$ for an appropriate μ.)

List of Symbols

A^*		142
$AC[0, 1]$		254
$\mathbb{C}$	the complex numbers	
c_0		69
$C(X)$		102
$C_{\mathbb{R}}(X)$		101, 102
$C_\infty(X)$		111
$C_0^\infty(\mathbb{R}^n)$		145
$d(\cdot, \cdot)$		4
$D(\cdot)$	(domain)	249
$\mathscr{D}_\Omega, \mathscr{D}_{\mathbb{R}^n}, \mathscr{D}$		147
$\mathscr{D}'_\Omega, \mathscr{D}'_{\mathbb{R}^n}, \mathscr{D}'$		148
$\mathscr{D}_{L^\infty(\mathbb{R}^n)}$		178
$\mathscr{E}, \mathscr{E}'$		178
$\check{f}, \hat{f}$		318
$f(A)$	(continuous functional calculus)	222
$f * g$		323
F_σ		31
$\mathscr{F}(\mathscr{H}), \mathscr{F}_s(\mathscr{H}), \mathscr{F}_s(\mathscr{H})$		53, 54
$\mathscr{F}, \mathscr{F}^{-1}$		318
G_δ		31, 105
$H_n(X)$	(homology group)	364
$\mathscr{H}$		39
$\mathscr{H}_{pp}, \mathscr{H}_{ac}, \mathscr{H}_{sing}$		230
$\mathscr{I}_1$		207
$\mathscr{I}_2$		208
Ker		185
l.s.c.		355
ℓ_2		40
ℓ_p		69
ℓ_∞		69
L^1		17
L^2		39
L^∞		67
$L^p(X, d\mu)$		68
$L^2(X, d\mu; \mathscr{H})$		40
$L^p(M, d\mu; E)$		89
$\mathscr{L}^1$		16
$\mathscr{L}(\mathscr{H})$		182
$\mathscr{L}(X, Y)$		69
$\mathscr{L}_\mathscr{H}$		310
$\mathscr{M}(X), \mathscr{M}_+(X), \mathscr{M}_{+,1}(X)$		109
$\mathscr{O}_D$		127
O_M^n		137
$P_\Omega(A), P_\Omega^A$		234
$\mathscr{P}\left(\frac{1}{x}\right)$		136
$Q(q)$		276
$\mathbb{R}$	the real numbers	
$R_\lambda(T)$	(resolvent)	188
Ran		185
s		69
$\mathscr{S}(\mathbb{R}^n)$		133
$\mathscr{S}'(\mathbb{R}^n)$		134
$\mathrm{tr}(\cdot)$		207, 212

$\beta(F, E)$	165	$\oplus$		40, 78
$\Gamma(T)$ (graph)	250	$\otimes$	(measures)	26
$\Gamma(\cdot)$	309	$\otimes$	(Hilbert spaces)	49
$d\Gamma(\cdot)$	302	$\otimes$	(functions)	141
$\eta(E^{**}, E)$	180	$\otimes$	(operators)	299
$\kappa(X)$	111			
μ_ψ	225			
$\rho(T)$	188	$\leqq$	(quadratic forms)	373
$\sigma(T)$	188	$\overline{\ }$	(closure)	92
$\sigma(X, Y)$	113	$^\circ$	(interior)	92
$\sigma_{pp}, \sigma_{cont}, \sigma_{ac}, \sigma_{sing}$	231	$^\circ$	(polar)	167
$\sigma_{disc}, \sigma_{ess}$	236	*	(adjoint)	187
$\tau(X, Y)$	163	*	(dual space)	72
ϕ_n (Hermite functions)	143	*	(convolution)	323
χ_A	2	$'$	(adjoint)	185
		Δ	(symmetric difference)	66
		$\xrightarrow{\|\cdot\|}, \xrightarrow{w}, \xrightarrow{s}$		182, 183
		$\|\cdot\|$	(absolute value of an operator)	196
$\|\cdot\|$	8	$^\perp$	(orthogonal complement)	41
$\|\cdot\|_1$	9	$\setminus$	(set difference)	1
$\|\cdot\|_\infty$	9	$/$	(quotient)	78, 79
$\|\cdot\|_{\alpha,\beta}$	133	$\langle\cdot,\cdot\rangle$	(ordered pair)	1
$\|\cdot\|_{\alpha,\beta,2}$	141	$(\cdot,\cdot)$	(inner product)	36
$\|\cdot\|_{\alpha,\beta,\infty}$	141			

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METHODS OF MODERN MATHEMATICAL PHYSICS

II: FOURIER ANALYSIS, SELF-ADJOINTNESS

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To our parents
Helen and Gerald Reed
Minnie and Hy Simon

Preface

This volume continues our series of texts devoted to functional analysis methods in mathematical physics. In Volume I we announced a table of contents for Volume II. However, in the preparation of the material it became clear that we would be unable to treat the subject matter in sufficient depth in one volume. Thus, the volume contains Chapters IX and X; we expect that a third volume will appear in the near future containing the rest of the material announced as "Analysis of Operators." We hope to continue this series with an additional volume on algebraic methods.

It gives us pleasure to thank many individuals:

E. Nelson for a critical reading of Chapter X; W. Beckner, H. Kalf, R. S. Phillips, and A. S. Wightman for critically reading one or more sections.

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Jackie and Martha for their encouragement and understanding.

MIKE REED
BARRY SIMON

June 1975

Introduction

A functional analyst is an analyst, first and foremost, and not a degenerate species of topologist.
E. Hille

Most texts in functional analysis suffer from a serious defect that is shared to an extent by Volume I of Methods of Modern Mathematical Physics. Namely, the subject is presented as an abstract, elegant corpus generally divorced from applications. Consequently, the students who learn from these texts are ignorant of the fact that almost all deep ideas in functional analysis have their *immediate* roots in "applications," either to classical areas of analysis such as harmonic analysis or partial differential equations, or to another science, primarily physics. For example, it was classical electromagnetic potential theory that motivated Fredholm's work on integral equations and thereby the work of Hilbert, Schmidt, Weyl, and Riesz on the abstractions of Hilbert space and compact operator theory. And it was the impetus of quantum mechanics that led von Neumann to his development of unbounded operators and later to his work on operator algebras.

More deleterious than historical ignorance is the fact that students are too often misled into believing that the most profitable directions for research in functional analysis are the abstract ones. In our opinion, exactly the opposite is true. We do not mean to imply that abstraction has no role to play. Indeed, it has the critical role of taking an idea from a concrete situation and, by eliminating the extraneous notions, making the idea more easily understood as well as applicable to a broader range of

situations. But it is the study of specific applications and the consequent generalizations that have been the more important, rather than the consideration of abstract questions about abstract objects for their own sake.

This volume contains a mixture of abstract results and applications, while the next contains mainly applications. The intention is to offer the readers of the whole series a properly balanced view.

We hope that this volume will serve several purposes: to provide an introduction for graduate students not previously acquainted with the material, to serve as a reference for mathematical physicists already working in the field, and to provide an introduction to various advanced topics which are difficult to understand in the literature. Not all the techniques and applications are treated in the same depth. In general, we give a very thorough discussion of the mathematical techniques and applications in quantum mechanics, but provide only an introduction to the problems arising in quantum field theory, classical mechanics, and partial differential equations. Finally, some of the material developed in this volume will not find application until Volume III. For all these reasons, this volume contains a great variety of subject matter. To help the reader select which material is important for him, we have provided a "Reader's Guide" at the end of each chapter.

As in Volume I, each chapter contains a section of notes. The notes give references to the literature and sometimes extend the discussion in the text. Historical comments are always limited by the knowledge and prejudices of authors, but in mathematics that arises directly from applications, the problem of assigning credit is especially difficult. Typically, the history is in two stages: first a specific method (typically difficult, computational, and sometimes nonrigorous) is developed to handle a small class of problems. Later it is recognized that the method contains ideas which can be used to treat other problems, so the study of the method itself becomes important. The ideas are then abstracted, studied on the abstract level, and the techniques systematized. With the newly developed machinery the original problem becomes an easy special case. In such a situation, it is often not completely clear how many of the mathematical ideas were already contained in the original work. Further, how one assigns credit may depend on whether one first learned the technique in the old computational way or in the new easier but more abstract way. In such situations, we hope that the reader will treat the notes as an introduction to the literature and not as a judgment of the historical value of the contributions in the papers cited.

Each chapter ends with a set of problems. As in Volume I, parts of proofs are occasionally left to the problems to encourage the reader to

participate in the development of the mathematics. Problems that fill gaps in the text are marked with a dagger. Difficult problems are marked with an asterisk. We strongly urge students to work the problems since that is the best way to learn mathematics.

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IX: The Fourier Transform

We have therefore the equation of condition

$$F(x) = \int dq\, Q \cos qx$$

If we substituted for Q any function of q, and conducted the integration from $q = 0$ to $q = \infty$, we should find a function of x: it is required to solve the inverse problem, that is to say, to ascertain what function of q, after being substituted for Q, gives as a result the function F(x), a remarkable problem whose solution demands attentive examination. *Joseph Fourier*

IX.1 The Fourier transform on $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{S}'(\mathbb{R}^n)$, convolutions

The Fourier transform is an important tool of both classical and modern analysis. We begin by defining it, and the inverse transform, on $\mathscr{S}(\mathbb{R}^n)$, the Schwartz space of C^∞ functions of rapid decrease.

Definition Suppose $f \in \mathscr{S}(\mathbb{R}^n)$. The **Fourier transform** of f is the function $\hat{f}$ given by

$$\hat{f}(\lambda) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ix\cdot\lambda} f(x)\, dx$$

where $x \cdot \lambda = \sum_{i=1}^n x_i \lambda_i$. The **inverse Fourier transform** of f, denoted by $\check{f}$, is the function

$$\check{f}(\lambda) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{ix\cdot\lambda} f(x)\, dx$$

We will occasionally write $\hat{f} = \mathscr{F}f$.

Since every function in Schwartz space is in $L^1(\mathbb{R}^n)$, the above integrals make sense. Many authors begin by discussing the Fourier transform on $L^1(\mathbb{R}^n)$. We start with Schwartz space for two reasons: First, the Fourier transform is a one-to-one map of Schwartz space onto itself (Theorem IX.1). This makes it particularly easy to talk about the inverse Fourier transform, which of course turns out to be the inverse map. That is, on Schwartz space, it is possible to deal with the transform and the inverse transform on an equal footing. Though this is also true for the Fourier transform on $L^2(\mathbb{R}^n)$ (see Theorem IX.6), it is not possible to define the Fourier transform on $L^2(\mathbb{R}^n)$ directly by the integral formula since $L^2(\mathbb{R}^n)$ functions may not be in $L^1(\mathbb{R}^n)$; a limiting procedure must be used. Secondly, once we know that the Fourier transform is a one-to-one, bounded map of $\mathscr{S}(\mathbb{R}^n)$ onto $\mathscr{S}(\mathbb{R}^n)$, we can easily extend it to $\mathscr{S}'(\mathbb{R}^n)$. It is this extension that is fundamental to the applications in Sections 5, 6, and 8.

We will use the standard multi-index notation. A multi-index

$$\alpha = \langle \alpha_1, \ldots, \alpha_n \rangle$$

is an n-tuple of nonnegative integers. The collection of all multi-indices will be denoted by I_+^n. The symbols $|\alpha|$, x^α, D^α, and x^2 are defined as follows:

$$|\alpha| = \sum_{i=1}^{n} \alpha_i$$

$$x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}$$

$$D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \cdots \partial x_n^{\alpha_n}}$$

$$x^2 = \sum_{i=1}^{n} x_i^2$$

In preparation for the proof that $\hat{}$ and $\check{}$ are inverses, we prove:

Lemma The maps $\hat{}$ and $\check{}$ are continuous linear transformations of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$. Furthermore, if α and β are multi-indices, then

$$((i\lambda)^\alpha D^\beta \hat{f})(\lambda) = \widehat{D^\alpha((-ix)^\beta f(x))} \tag{IX.1}$$

Proof The map $\hat{}$ is clearly linear. Since

$$\begin{aligned}(\lambda^\alpha D^\beta \hat{f})(\lambda) &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \lambda^\alpha (-ix)^\beta e^{-i\lambda\cdot x} f(x)\, dx \\ &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \frac{1}{(-i)^\alpha} (D_x^\alpha e^{-i\lambda\cdot x})(-ix)^\beta f(x)\, dx \\ &= \frac{(-i)^\alpha}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\lambda\cdot x} D_x^\alpha((-ix)^\beta f(x))\, dx\end{aligned}$$

We conclude that

$$\|\hat{f}\|_{\alpha,\beta} = \sup_{\lambda} |\lambda^\alpha (D^\beta \hat{f})(\lambda)| \leq \frac{1}{(2\pi)^{n/2}} \int |D_x^\alpha (x^\beta f)| \, dx < \infty$$

so $\hat{}$ takes $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$, and we have also proven (IX.1). Furthermore, if k is large enough, $\int (1+x^2)^{-k} \, dx < \infty$ so that

$$\|\hat{f}\|_{\alpha,\beta} \leq \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \frac{(1+x^2)^{-k}}{(1+x^2)^{-k}} |D_x^\alpha (-ix)^\beta f(x)| \, dx$$

$$\leq \frac{1}{(2\pi)^{n/2}} \left(\int (1+x^2)^{-k} \, dx \right) \sup_x \{(1+x^2)^{+k} |D_x^\alpha (-ix)^\beta f(x)|\}$$

Using Leibnitz's rule we easily conclude that there exist multi-indices α_j, β_j and constants c_j so that

$$\|\hat{f}\|_{\alpha,\beta} \leq \sum_{j=1}^{M} c_j \|f\|_{\alpha_j,\beta_j}$$

Thus, $\hat{}$ is bounded and by Theorem V.4 is therefore continuous. The proof for $\check{}$ is the same. ∎

We are now ready to prove the Fourier inversion theorem. The proof we give uses the original idea of Fourier.

Theorem IX.1 (Fourier inversion theorem) The Fourier transform is a linear bicontinuous bijection from $\mathscr{S}(\mathbb{R}^n)$ onto $\mathscr{S}(\mathbb{R}^n)$. Its inverse map is the inverse Fourier transform, i.e., $\check{\hat{f}} = f = \hat{\check{f}}$.

Proof We will prove that $\check{\hat{f}} = f$. The proof that $\hat{\check{f}} = f$ is similar. $\hat{\check{f}} = f$ implies that $\hat{}$ is surjective and $\check{\hat{f}} = f$ implies that $\hat{}$ is injective. Since $\hat{}$ and $\check{}$ are continuous maps of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$, it is sufficient to prove that $\check{\hat{f}} = f$ for f contained in the dense set $C_0^\infty(\mathbb{R}^n)$. Let C_ε be the cube of volume $(2/\varepsilon)^n$ centered at the origin in $\mathbb{R}^n$. Choose ε small enough so that the support of f is contained in C_ε. Let

$$K_\varepsilon = \{\mathbf{k} \in \mathbb{R} \mid \text{each } k_i/\pi\varepsilon \text{ is an integer}\}$$

Then

$$f(x) = \sum_{k \in K_\varepsilon} ((\tfrac{1}{2}\varepsilon)^{n/2} e^{ik \cdot x}, f)(\tfrac{1}{2}\varepsilon)^{n/2} e^{ik \cdot x}$$

is just the Fourier series of f which converges uniformly in C_ε to f since f is continuously differentiable (Theorem II.8). Thus

$$f(x) = \sum_{k \in K_\varepsilon} \frac{\hat{f}(k) e^{ik \cdot x}}{(2\pi)^{n/2}} (\pi\varepsilon)^n \tag{IX.2}$$

Since $\mathbb{R}^n$ is the disjoint union of the cubes of volume $(\pi\varepsilon)^n$ centered about the points in K_ε, the right-hand side of (IX.2) is just a Riemann sum for the integral of the function $\hat{f}(k)e^{ik\cdot x}/(2\pi)^{n/2}$. By the lemma, $\hat{f}(k)e^{ik\cdot x} \in \mathscr{S}(\mathbb{R}^n)$, so the Riemann sums converge to the integral. Thus $\check{\hat{f}} = f$. ∎

Corollary Suppose $f \in \mathscr{S}(\mathbb{R}^n)$. Then

$$\int_{\mathbb{R}^n} |f(x)|^2\, dx = \int_{\mathbb{R}^n} |\hat{f}(k)|^2\, dk$$

Proof This is really a corollary of the proof rather than the statement of Theorem IX.1. If f has compact support, then for ε small enough,

$$f(x) = \sum_{k \in K_\varepsilon} ((\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x},\ f(x))(\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}$$

Since $\{(\frac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}\}_{k \in K_\varepsilon}$ is an orthonormal basis for $L^2(C_\varepsilon)$,

$$\begin{aligned}
\int_{\mathbb{R}^n} |f(x)|^2\, dx &= \int_{C_\varepsilon} |f(x)|^2\, dx \\
&= \sum_{k \in K_\varepsilon} |((\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x},\ f(x))|^2 \\
&= \sum_{k \in K_\varepsilon} |\hat{f}(k)|^2 (\pi\varepsilon)^n \\
&\xrightarrow[\varepsilon \to 0]{} \int_{\mathbb{R}^n} |\hat{f}(k)|^2\, dk
\end{aligned}$$

This proves the corollary for $f \in C_0^\infty$. Since $\hat{\ }$ and $\|\cdot\|_2$ are continuous on $\mathscr{S}$ and C_0^∞ is dense, the result holds for all of $\mathscr{S}$. ∎

Example 1 We compute the Fourier transform of $f(x) = e^{-\alpha x^2/2} \in \mathscr{S}(\mathbb{R})$ where $\alpha > 0$.

$$\begin{aligned}
\hat{f}(\lambda) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-\alpha x^2/2} e^{-i\lambda\cdot x}\, dx \\
&= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \sqrt{\frac{2}{\alpha}} \exp\left(-t^2 - it\lambda\sqrt{\frac{2}{\alpha}}\right) dt \\
&= \frac{e^{-\lambda^2/2\alpha}}{\sqrt{\alpha\pi}} \int_{\mathbb{R}} \exp -\left(t + i\frac{\lambda}{\sqrt{2\alpha}}\right)^2 dt \\
&= \frac{e^{-\lambda^2/2\alpha}}{\sqrt{\alpha\pi}} \int_{\mathbb{R}} e^{-t^2}\, dt = \frac{e^{-\lambda^2/2\alpha}}{\sqrt{\alpha}}
\end{aligned}$$

The next to last step follows from the Cauchy integral formula and the exponential decrease of e^{-z^2} along lines parallel to the x axis.

We now define the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$.

Definition Let $T \in \mathscr{S}'(\mathbb{R}^n)$. Then the Fourier transform of T, denoted by $\hat{T}$, is the tempered distribution defined by $\hat{T}(\varphi) = T(\hat{\varphi})$.

Suppose that $h, \varphi \in \mathscr{S}(\mathbb{R}^n)$, then by the polarization identity and the corollary to Theorem IX.1 we have $(h, \varphi) = (\hat{h}, \hat{\varphi})$. Substituting $\bar{\hat{g}} = \check{\bar{g}}$ for h, we obtain

$$T_{\hat{g}}(\varphi) = \int \hat{g}(x)\varphi(x)\,dx = \int g(x)\hat{\varphi}(x)\,dx = T_g(\hat{\varphi}) = \hat{T}_g(\varphi)$$

where $T_{\hat{g}}$ and T_g are the distributions corresponding to the functions $\hat{g}$ and g respectively. This shows that the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$ extends the transform we previously defined on $\mathscr{S}(\mathbb{R}^n)$.

Theorem IX.2 The Fourier transform is a one-to-one linear bijection from $\mathscr{S}'(\mathbb{R}^n)$ to $\mathscr{S}'(\mathbb{R}^n)$ which is the unique weakly continuous extension of the Fourier transform on $\mathscr{S}(\mathbb{R}^n)$.

Proof If $\varphi_n \xrightarrow{\mathscr{S}} \varphi$, then by Theorem IX.1, $\hat{\varphi}_n \xrightarrow{\mathscr{S}} \hat{\varphi}$, so $T(\hat{\varphi}_n) \to T(\hat{\varphi})$ for each T in $\mathscr{S}'(\mathbb{R}^n)$. Thus $\hat{T}(\varphi_n) \to \hat{T}(\varphi)$, which shows that $\hat{T}$ is a continuous linear functional on $\mathscr{S}(\mathbb{R}^n)$. Furthermore, if $T_n \xrightarrow{w} T$, then $\hat{T}_n \xrightarrow{w} \hat{T}$ because $T_n(\hat{\varphi}) \to T(\hat{\varphi})$ implies $\hat{T}_n(\varphi) \to \hat{T}(\varphi)$. Thus $T \mapsto \hat{T}$ is weakly continuous.

The remaining properties of $\hat{}$ follow immediately from the corresponding statements on $\mathscr{S}(\mathbb{R}^n)$ (see Problem 19 in Chapter V). ∎

Example 2 We compute the Fourier transform of the derivative of the delta function at $b \in \mathbb{R}$:

$$\begin{aligned}
\hat{\delta}_b'(\varphi) &= \delta_b'(\hat{\varphi}) \\
&= \delta_b\left(-\frac{d}{d\lambda}\hat{\varphi}(\lambda)\right) \\
&= \delta_b\left(\frac{-1}{(2\pi)^{1/2}}\int e^{-i\lambda x}(-ix)\varphi(x)\,dx\right) \\
&= \int \left(\frac{ixe^{-ibx}}{\sqrt{2\pi}}\right)\varphi(x)\,dx
\end{aligned}$$

So, the Fourier transform of δ_b' is the function $ixe^{-ibx}/\sqrt{2\pi}$.

* * *

We now introduce a new operation on functions.

Definitions Suppose that $f, g \in \mathscr{S}(\mathbb{R}^n)$. Then the **convolution** of f and g, denoted by $f * g$, is the function

$$(f * g)(y) = \int_{\mathbb{R}^n} f(y - x)g(x)\,dx$$

The convolution arises in many circumstances (we have already used it in discussing closed operators in Section VIII.1). In Section 4 we use interpolation theorems to prove L^p estimates on the convolution $f * g$ in terms of f and g. In this section we concentrate on the properties of the convolution as a map from $\mathscr{S}(\mathbb{R}^n) \times \mathscr{S}(\mathbb{R}^n)$ to $\mathscr{S}(\mathbb{R}^n)$. Using these properties we show that the convolution can be extended to a map from $\mathscr{S}'(\mathbb{R}^n) \times \mathscr{S}(\mathbb{R}^n)$ to O_M^n, the polynomially bounded C^∞ functions. Convolutions frequently occur when one uses the Fourier transform because the Fourier transform takes products into convolutions (Theorem IX.3b and Theorem IX.4c).

Theorem IX.3

(a) For each $f \in \mathscr{S}(\mathbb{R}^n)$, $g \to f * g$ is a continuous map of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$.

(b) $\widehat{fg} = (2\pi)^{-n/2}\hat{f} * \hat{g}$ and $\widehat{f * g} = (2\pi)^{n/2}\hat{f}\hat{g}$.

(c) For f, g, h, in $\mathscr{S}(\mathbb{R}^n)$, $f * g = g * f$ and $f * (g * h) = (f * g) * h$.

Proof From the polarization identity and the corollary to Theorem IX.1 we find that $(\varphi, \psi) = (\hat{\varphi}, \hat{\psi})$ for $\varphi, \psi \in \mathscr{S}(\mathbb{R}^n)$. Letting $y \in \mathbb{R}^n$ be fixed, we apply this identity to $e^{iy \cdot x}\overline{f}(x)$ and g obtaining $(e^{iy \cdot x}\overline{f}, g) = (\widehat{e^{iy \cdot x}\overline{f}}, \hat{g})$. But

$$(e^{iy \cdot x}\overline{f}, g) = \int_{\mathbb{R}^n} e^{-iy \cdot x} f(x)g(x)\,dx$$

and

$$(\widehat{e^{iy \cdot x}\overline{f}}, \hat{g}) = \int_{\mathbb{R}^n} \left(\overline{(2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i\lambda \cdot x + iy \cdot x} \overline{f(x)}\,dx} \right) \hat{g}(\lambda)\,d\lambda$$

$$= \int_{\mathbb{R}^n} \hat{f}(y - \lambda)\hat{g}(\lambda)\,d\lambda$$

which proves that $\widehat{fg} = (2\pi)^{-n/2}\hat{f} * \hat{g}$. Using the inverse Fourier transform this formula may be stated as

$$(2\pi)^{n/2}\widehat{f\check{g}} = f * g$$

This shows that convolution is the composition of the inverse Fourier transform, multiplication by $(2\pi)^{n/2}\check{f}$, and the Fourier transform. It follows that convolution is continuous.

The statements in (c) follow trivially from (b). ∎

In order to extend the map $C_f : g \to f * g$ to $\mathcal{S}'$, we look for a continuous map $\tilde{C}_f : \mathcal{S} \to \mathcal{S}$ so that $\tilde{C}_f' \restriction \mathcal{S} = C_f$. We then define $\tilde{C}_f'$ to be convolution on $\mathcal{S}'$.

Definition Suppose that $f \in \mathcal{S}(\mathbb{R}^n)$, $T \in \mathcal{S}'(\mathbb{R}^n)$ and let $\check{f}(x)$ denote the function, $f(-x)$. Then, the **convolution** of T and f, denoted $T * f$, is the distribution in $\mathcal{S}'(\mathbb{R}^n)$ given by

$$(T * f)(\varphi) = T(\check{f} * \varphi)$$

for all $\varphi \in \mathcal{S}(\mathbb{R}^n)$.

The fact that $g \to \check{f} * g$ is a continuous transformation guarantees that $T * f \in \mathcal{S}'(\mathbb{R}^n)$. The following theorem summarizes the properties of this extended convolution.

Let f_y denote the function $f_y(x) = f(x - y)$ and $\check{f}_y$ the function $f(y - x)$. When f is given by a large expression $(\cdots)$, we will sometimes write $(\cdots)^{\check{}}$ rather than $(\cdots\check{})$.

Theorem IX.4 For each $f \in \mathcal{S}(\mathbb{R}^n)$ the map $T \to T * f$ is a weakly continuous map of $\mathcal{S}'(\mathbb{R}^n)$ into $\mathcal{S}'(\mathbb{R}^n)$ which extends the convolution on $\mathcal{S}(\mathbb{R}^n)$. Furthermore,

(a) $T * f$ is a polynomially bounded C^∞ function, i.e. $T * f \in O_M^n$. In fact, $(T * f)(y) = T(\check{f}_y)$ and

$$D^\beta(T * f) = (D^\beta T) * f = T * D^\beta f \tag{IX.3}$$

(b) $(T * f) * g = T * (f * g)$

(c) $\widehat{T * f} = (2\pi)^{n/2} \hat{f} \hat{T}$

Proof Since $T \to T * f$ is defined as the adjoint of a bounded map from $\mathcal{S}$ to $\mathcal{S}$, it is automatically weakly continuous. The fact that it extends the convolution on $\mathcal{S}$ is just a change of variables. The statements (IX.3), (b), and (c), all follow immediately from the corresponding statements for $T \in \mathcal{S}$ and the facts that $\mathcal{S}$ is weakly dense in $\mathcal{S}'$ and that $\mathcal{F}$, D^β, multiplication by $\hat{f}$, and convolution are all weakly continuous on $\mathcal{S}'$.

It remains to prove the first part of (a). Since $T \in \mathscr{S}'(\mathbb{R}^n)$, it follows from the regularity theorem (Theorem V.10) that there is a bounded continuous function h, a positive integer r, and a multi-index β so that

$$T(\check{f}_y) = \int_{\mathbb{R}^n} h(x)(1 + x^2)^r (D^\beta f)(y - x)\, dx$$

Since $D^\beta f \in \mathscr{S}$, $T(\check{f}_y)$ is an infinitely differentiable function of y. The change of variables $\tau = y - x$ shows that

$$\begin{aligned} |T(\check{f}_y)| &\le \|h\|_\infty \int_{\mathbb{R}^n} (1 + x^2)^r |(D^\beta f)(y - x)|\, dx \\ &= \|h\|_\infty \int_{\mathbb{R}^n} (1 + (y - \tau)^2)^r |D^\beta f(\tau)|\, d\tau \end{aligned}$$

from which it follows easily that $y \mapsto T(\check{f}_y)$ is polynomially bounded. A similar proof works for the derivatives of $y \mapsto T(\check{f}_y)$. Thus $T(\check{f}_y) \in O_M^n$.

Suppose that a distribution $S \in \mathscr{S}'(\mathbb{R}^n)$ is given by a polynomially bounded continuous function s. Then, using Fubini's theorem we find that for $\varphi \in \mathscr{S}(\mathbb{R}^n)$

$$\begin{aligned} (S * f)(\varphi) &\equiv S(\check{f} * \varphi) \\ &= \int s(x) \left(\int \check{f}(x - y)\varphi(y)\, dy \right) dx \\ &= \int \left(\int s(x)\check{f}_y(x)\, dx \right) \varphi(y)\, dy \\ &= (S(\check{f}_y))(\varphi) \end{aligned}$$

so $S * f = S(\check{f}_y)$. By the regularity theorem $T = D^\alpha S$ for some such S. Thus by (IX.3)

$$\begin{aligned} T * f = (D^\alpha S) * f &= S * D^\alpha f \\ &= S((D^\alpha f)\check{}_y) \\ &= (-1)^{|\alpha|} S(D^\alpha(\check{f}_y)) \\ &= D^\alpha S(\check{f}_y) \\ &= T(\check{f}_y) \end{aligned}$$

This completes the proof. ∎

Theorem IX.5 Let $T \in \mathscr{S}'(\mathbb{R}^n)$ and $f \in \mathscr{S}(\mathbb{R}^n)$. Then $\widehat{fT} \in O_M^n$ and $\widehat{fT}(k) = (2\pi)^{-n/2} T(f e^{-ik\cdot x})$. In particular, if T has compact support and $\psi \in \mathscr{S}(\mathbb{R}^n)$ is identically one on a neighborhood of the support of T, then

$$\hat{T}(k) = (2\pi)^{-n/2} T(\psi e^{-ik\cdot x})$$

Proof By Theorem IX.4c and the Fourier inversion formula we have $\widehat{fT} = (2\pi)^{-n/2} \hat{f} * \hat{T}$. Thus $\widehat{fT} \in O_M^n$ and

$$\begin{aligned} \widehat{fT}(k) &= (2\pi)^{-n/2} \hat{T}(\tilde{f}_k) \\ &= (2\pi)^{-n/2} T(e^{-ik\cdot x} f) \end{aligned}$$

∎

We remark that one can also define the convolution of a distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ with an $f \in \mathscr{D}(\mathbb{R}^n)$ by $(T * f)(y) = T(\tilde{f}_y)$. A proof similar to the proof of Theorem IX.4 shows that $T * f$ is a (not necessarily polynomially bounded) C^∞ function and that (IX.3) holds.

We have already introduced the term "approximate identity" in Section VIII.1; we now define it formally.

Definition Let $j(x)$ be a positive C^∞ function whose support lies in the sphere of radius one about the origin in $\mathbb{R}^n$ and which satisfies $\int j(x)\,dx = 1$. The sequence of functions $j_\varepsilon(x) = \varepsilon^{-n} j(x/\varepsilon)$ is called an **approximate identity.**

Proposition Suppose $T \in \mathscr{S}'(\mathbb{R}^n)$ and let $j_\varepsilon(x)$ be an approximate identity. Then $T * j_\varepsilon \to T$ weakly as $\varepsilon \to 0$.

Proof If $\varphi \in \mathscr{S}(\mathbb{R}^n)$, then $(T * j_\varepsilon)(\varphi) = T(\tilde{j}_\varepsilon * \varphi)$, so it is sufficient to show that $\tilde{j}_\varepsilon * \varphi \xrightarrow{\mathscr{S}(\mathbb{R}^n)} \varphi$. To do this it is sufficient to show that $(2\pi)^{n/2} \hat{j}_\varepsilon \hat{\varphi} \xrightarrow{\mathscr{L}} \hat{\varphi}$. Since $\hat{j}_\varepsilon(\lambda) = \hat{j}(\varepsilon\lambda)$ and $\hat{j}(0) = (2\pi)^{-n/2}$, it follows that $(2\pi)^{n/2} \hat{j}_\varepsilon(x)$ converges to 1 uniformly on compact sets and is uniformly bounded. Similarly, $D^\alpha \hat{j}_\varepsilon$ converges uniformly to zero. We conclude that $(2\pi)^{n/2} \hat{j}_\varepsilon \hat{\varphi} \xrightarrow{\mathscr{L}} \hat{\varphi}$. ∎

IX.2 The range of the Fourier transform: Classical spaces

We have defined the Fourier transform on $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{S}'(\mathbb{R}^n)$. In this section, Section IX.3, and Section IX.9, we investigate the range of the Fourier transform when it is restricted to various subsets of $\mathscr{S}'(\mathbb{R}^n)$. These

questions are natural and have historical interest, but more important, characterizing the range of the Fourier transform is very useful. One is often able to obtain information about the Fourier transform of a function and one would like to know what this says about the function itself. We begin with two theorems which follow easily from the work that we have already done in Section IX.1.

Theorem IX.6 (the Plancherel theorem) The Fourier transform extends uniquely to a unitary map of $L^2(\mathbb{R}^n)$ onto $L^2(\mathbb{R}^n)$. The inverse transform extends uniquely to its adjoint.

Proof The corollary to Theorem IX.1 states that if $f \in \mathscr{S}(\mathbb{R}^n)$, then $\|f\|_2 = \|\hat{f}\|_2$. Since $\mathscr{F}[\mathscr{S}] = \mathscr{S}$, $\mathscr{F}$ is a surjective isometry on $L^2(\mathbb{R}^n)$. ∎

Theorem IX.7 (the Riemann–Lebesgue lemma) The Fourier transform extends uniquely to a bounded map from $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$, the continuous functions vanishing at ∞.

Proof For $f \in \mathscr{S}(\mathbb{R}^n)$, we know that $\hat{f} \in \mathscr{S}(\mathbb{R}^n)$ and thus $\hat{f} \in C_\infty(\mathbb{R}^n)$. The estimate

$$\|\hat{f}\|_\infty \leq (2\pi)^{-n/2}\|f\|_1$$

is trivial. The Fourier transform is thus a bounded linear map from a dense set of $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$. By the B.L.T. theorem, $\hat{}$ extends uniquely to a bounded linear transformation of $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$. ∎

We remark that the Fourier transform takes $L^1(\mathbb{R}^n)$ into, but not onto $C_\infty(\mathbb{R}^n)$ (Problem 16).

A simple argument with test functions shows that the extended transform on $L^1(\mathbb{R}^n)$ and $L^2(\mathbb{R}^n)$ is the restriction of the transform on $\mathscr{S}'(\mathbb{R}^n)$, but it is useful to have an explicit integral representation. For $f \in L^1(\mathbb{R}^n)$, this is easy since we can find $f_m \in \mathscr{S}(\mathbb{R}^n)$ so that $\|f - f_m\|_1 \to 0$. Then, for each λ,

$$\begin{aligned}\hat{f}(\lambda) &= \lim_{m\to\infty} (\hat{f}_m(\lambda)) \\ &= \lim_{m\to\infty} \left\{ \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\lambda\cdot x} f_m(x)\, dx \right\} \\ &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\lambda\cdot x} f(x)\, dx\end{aligned}$$

So, the Fourier transform of a function in $L^1(\mathbb{R}^n)$ is given by the usual formula.

Next, suppose $f \in L^2(\mathbb{R}^n)$ and let

$$\chi_R(x) = \begin{cases} 1 & |x| \leq R \\ 0 & |x| > R \end{cases}$$

Then $\chi_R f \in L^1(\mathbb{R}^n)$ and $\chi_R f \xrightarrow[R\to\infty]{L^2} f$, so by the Plancherel theorem $\widehat{\chi_R f} \xrightarrow[R\to\infty]{L^2} \hat{f}$. For $\chi_R f$ we have the usual formula; thus

$$\hat{f}(\lambda) = \underset{R\to\infty}{\text{l.i.m.}} (2\pi)^{-n/2} \int_{|x|\leq R} e^{-i\lambda\cdot x} f(x)\, dx$$

where by "l.i.m." we mean the limit in the L^2-norm. Sometimes we will dispense with $|x| \leq R$ and just write

$$\hat{f}(\lambda) = \text{l.i.m.} (2\pi)^{-n/2} \int e^{-i\lambda\cdot x} f(x)\, dx$$

for functions $f \in L^2(\mathbb{R}^n)$.

We have proven above that $L^2(\mathbb{R}^n) \xrightarrow{\hat{}} L^2(\mathbb{R}^n)$ and $L^1(\mathbb{R}^n) \xrightarrow{\hat{}} L^\infty(\mathbb{R}^n)$ and in both cases $\hat{}$ is a bounded operator. It is exactly in situations like this that one can use the interpolation theorems which we will prove in the Appendix to Section 4.

Theorem IX.8 (Hausdorff–Young inequality) Suppose $1 \leq q \leq 2$, and $p^{-1} + q^{-1} = 1$. Then the Fourier transform is a bounded map of $L^q(\mathbb{R}^n)$ to $L^p(\mathbb{R}^n)$ and its norm is less than or equal to $(2\pi)^{n(1/2-1/q)}$.

Proof We use the Riesz–Thorin theorem (Theorem IX.17) with $q_0 = 2 = p_0$, $p_1 = \infty$, and $q_1 = 1$. Since $\|\hat{f}\|_2 = \|f\|_2$ and $\|\hat{f}\|_\infty \leq (2\pi)^{-n/2}\|f\|_1$, we conclude that $\|\hat{f}\|_{p_t} \leq C_t \|f\|_{q_t}$ where $p_t^{-1} = (1-t)/2$, $q_t^{-1} = (1-t)/2 + t = 1 - p_t^{-1}$, and $\log C_t = t \log(2\pi)^{-n/2}$. ∎

* * *

We now come to another natural question. What are the Fourier transforms of the finite positive measures on $\mathbb{R}^n$? Suppose that we define

$$\hat{\mu}(\lambda) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i\lambda\cdot x}\, d\mu(x)$$

Then, if $\varphi \in \mathscr{S}(\mathbb{R}^n)$,

$$\begin{aligned}\int_{\mathbb{R}^n} \hat{\mu}(\lambda)\varphi(\lambda)\, d\lambda &= (2\pi)^{-n/2} \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} e^{-i\lambda \cdot x}\, d\mu(x) \right) \varphi(\lambda)\, d\lambda \\ &= (2\pi)^{-n/2} \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} e^{-i\lambda \cdot x} \varphi(\lambda)\, d\lambda \right) d\mu(x) \\ &= \int_{\mathbb{R}^n} \hat{\varphi}(x)\, d\mu(x)\end{aligned}$$

so this definition coincides with the restriction of the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$ to the positive measures. Suppose $\lambda_1, \ldots, \lambda_N \in \mathbb{R}^n$ and $\xi = \langle \xi_1, \xi_2, \ldots, \xi_N \rangle \in \mathbb{C}^N$. Then

$$\sum_{i,j=1}^{N} \hat{\mu}(\lambda_i - \lambda_j)\bar{\xi}_j \xi_i = \int \left| \sum_{i=1}^{N} \xi_i e^{-i\lambda_i \cdot x} \right|^2 d\mu(\mathbf{x}) \geq 0$$

This shows that the function $\hat{\mu}(\lambda)$ has the property that for any $\lambda_1, \ldots, \lambda_N \in \mathbb{R}^n$, $\{\hat{\mu}(\lambda_i - \lambda_j)\}$ is the matrix of a positive operator on $\mathbb{C}^N$. Furthermore, by the dominated convergence theorem, $\hat{\mu}$ is continuous, and since

$$\begin{aligned}|\hat{\mu}(\lambda)| &\leq (2\pi)^{-n/2} \int_{\mathbb{R}^n} |e^{-i\lambda \cdot x}|\, d\mu(\mathbf{x}) \\ &= (2\pi)^{-n/2} \mu(\mathbb{R}^n)\end{aligned}$$

$\hat{\mu}(\cdot)$ is also bounded.

Definition A complex-valued, bounded, continuous function f on $\mathbb{R}^n$ that has the property that $\{f(\lambda_i - \lambda_j)\}_{i,j}$ is a positive matrix on $\mathbb{C}^N$ for each N and all $\lambda_1, \ldots, \lambda_N \in \mathbb{R}^n$ is called a **function of positive type.**

There are three properties of functions of positive type which follow easily from the definition. Letting $N = 1$, $x \in \mathbb{R}^N$,

$$(1) \quad f(0) \geq 0$$

since $f(0)$ is a positive operator on $\mathbb{C}^1$. Letting $N = 2$, and choosing $\lambda_1 = x$, $\lambda_2 = 0$, we see that the matrix

$$\begin{pmatrix} f(0) & f(x) \\ f(-x) & f(0) \end{pmatrix}$$

must be positive and therefore self-adjoint with positive determinant. This implies that

$$(2) \quad f(x) = \overline{f(-x)}$$
$$(3) \quad |f(x)| \leq f(0)$$

Notice that in proving these three properties we did not use the fact that $f(x)$ is bounded, so we could have left out the word *bounded* in the definition and recovered boundedness from (3) above. It is clear that any convex combinations or scalar multiples of functions of positive type again give functions of positive type, so these functions form a cone.

Theorem IX.9 (Bochner's theorem) The set of Fourier transforms of the finite, positive measures on $\mathbb{R}^n$ is exactly the cone of functions of positive type.

Proof We do not give Bochner's original proof but rather an easy, interesting argument based on Stone's theorem. We have already shown that the Fourier transforms of finite positive measures are functions of positive type. We need to prove the converse. Suppose f is of positive type. Let $\mathscr{K}$ denote the set of complex-valued functions on $\mathbb{R}^n$ which vanish except at a finite number of points. Then

$$(\psi, \varphi)_f = \sum_{\mathbf{x}, \mathbf{y} \in \mathbb{R}^n} f(\mathbf{x} - \mathbf{y})\overline{\psi(\mathbf{x})}\varphi(\mathbf{y})$$

has all the properties of a well-defined inner product except that we may have $(\varphi, \varphi)_f = 0$ for some $\varphi \neq 0$. If we let $\mathscr{N}$ be the set of such φ, then $\mathscr{K}/\mathscr{N}$ is a well-defined pre-Hilbert space under $(\cdot, \cdot)_f$. Suppose that $\mathbf{t} \in \mathbb{R}^n$ and define $U_\mathbf{t}$ on $\mathscr{K}$ by $(U_\mathbf{t}\varphi)(\mathbf{x}) = \varphi(\mathbf{x} - \mathbf{t})$. Since $U_\mathbf{t}$ preserves the form $(\cdot, \cdot)_f$, it takes equivalence classes into equivalence classes and thus restricts to an isometry on $\mathscr{K}/\mathscr{N}$. Since the same is true of $U_{-\mathbf{t}}$, this isometry has dense range and thus extends to a unitary operator $\tilde{U}_\mathbf{t}$ on $\mathscr{H} = \overline{\mathscr{K}/\mathscr{N}}$. Furthermore, $\tilde{U}_{\mathbf{t}+\mathbf{s}} = \tilde{U}_\mathbf{t}\tilde{U}_\mathbf{s}$, $\tilde{U}_\mathbf{0} = I$, and because of the continuity of f, $\tilde{U}_\mathbf{t}$ is strongly continuous. Thus the map $\mathbf{t} \to \tilde{U}_\mathbf{t}$ satisfies the hypotheses of Theorem VIII.12 (the generalization of Stone's theorem). Therefore, there is a projection-valued measure P_λ, on $\mathbb{R}^n$ so that

$$(\varphi, \tilde{U}_\mathbf{t}\psi)_f = \int_{\mathbb{R}^n} e^{i\mathbf{t}\cdot\lambda}\, d(\varphi, P_\lambda\psi)_f$$

Let $\tilde{\varphi}_\mathbf{0}$ denote the equivalence class containing the function

$$\varphi_\mathbf{0}(\mathbf{x}) = \begin{cases} 1, & x = 0 \\ 0, & x \neq 0 \end{cases}$$

Then

$$f(\mathbf{t}) = \tilde{U}_\mathbf{t}\tilde{\varphi}_\mathbf{0}, \tilde{\varphi}_\mathbf{0})_f = (\tilde{\varphi}_\mathbf{0}, \tilde{U}_{-\mathbf{t}}\tilde{\varphi}_\mathbf{0})_f = \int e^{-i\mathbf{t}\cdot\lambda}\, d(\tilde{\varphi}_\mathbf{0}, P_\lambda\tilde{\varphi}_\mathbf{0})_f$$

so we have displayed f as the Fourier transform of a finite positive measure. ∎

The notion of positive type may be generalized to distributions. If $f(x)$ is a bounded continuous function, then $f(x)$ will be of positive type if and only if

$$\int\int f(x-y)\overline{\varphi(y)}\varphi(x)\,dx\,dy \geq 0 \tag{IX.4}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^n)$. To see this one need only approximate the integral in (IX.4) by a Riemann sum. This condition can be rewritten as

$$\iint f(\tau)\overline{\varphi(x-\tau)}\varphi(x)\,d\tau\,dx = \int f(\tau)(\tilde{\bar{\varphi}} * \varphi)(\tau)\,d\tau \geq 0 \tag{IX.5}$$

where $\tilde{\varphi}$ is the function $\tilde{\varphi}(x) = \varphi(-x)$. This suggests the following definition.

Definition A distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ is said to be of **positive type** if $T(\tilde{\bar{\varphi}} * \varphi) \geq 0$ for all $\varphi \in \mathscr{D}(\mathbb{R}^n)$.

The following generalization of Bochner's theorem is due to Schwartz. This theorem is particularly interesting since it implies that certain ordinary distributions must be tempered. The proof is sketched in Problem 20 (or see the Notes for a reference).

Theorem IX.10 (the Bochner–Schwartz theorem) A distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ is a distribution of positive type if and only if $T \in \mathscr{S}'(\mathbb{R}^n)$ and T is the Fourier transform of a positive measure of at most polynomial growth.

If $f(x)$ is a function of positive type, then this theorem implies that the weak derivatives $(-\Delta)^m f$ are all distributions of positive type. For $\hat{f} = \mu$, a finite measure by Theorem IX.9, and $\widehat{(-\Delta)^m f} = |x|^{2m}\mu$, a positive measure of polynomial growth.

Finally, we determine which bounded measurable functions are distributions of positive type. A bounded measurable function f on $\mathbb{R}^n$ is said to be of **weak positive type** if (IX.4) holds. Since (IX.5) follows from (IX.4), the distribution

$$T_f(\varphi) = \int f(x)\varphi(x)\,dx$$

is of positive type and therefore $\hat{T}_f = \mu$, a polynomially bounded positive

measure. If $j_\varepsilon(x)$ is an approximate identity that is symmetric about the origin, then

$$\begin{aligned}\|f\|_\infty \geq T_f(j_\varepsilon * j_\varepsilon) &= \hat{T}_f(\widehat{(j_\varepsilon * j_\varepsilon)}) \\ &= (2\pi)^{n/2}\mu(|\check{j}_\varepsilon(x)|^2) \\ &= (2\pi)^{n/2}\int |\check{j}_\varepsilon(x)|^2\, d\mu(x)\end{aligned}$$

On each compact subset of $\mathbb{R}^n$, $\check{j}_\varepsilon(x)$ converges uniformly to $(2\pi)^{-n/2}$ as $\varepsilon \to 0$, so the μ-measure of any compact set is less than $(2\pi)^{n/2}\|f\|_\infty$, so μ is finite.

We now come to the interesting point. Since μ is finite, its Fourier transform is a continuous function of positive type. Since μ and f must coincide a.e., we have proven:

Proposition A bounded function of weak positive type is equal almost everywhere to a continuous function of positive type.

IX.3 The range of the Fourier transform: Analyticity

In this section we investigate the connection between the decay properties of a function or distribution at infinity and the analyticity properties of its Fourier transform. The most extreme form of decay at infinity is to have compact support. We will prove the Paley–Wiener and Schwartz theorems which characterize explicitly the Fourier transforms of C^∞ functions and distributions with compact support. We then state two theorems relating exponential decay to analyticity properties of the Fourier transform. We close the section by characterizing the Fourier transforms of tempered distributions whose supports lie in symmetric cones. There are many other theorems of this genre; some of them are discussed in the Notes.

Suppose that $f \in C_0^\infty(\mathbb{R}^n)$. Then for all $\zeta = \langle \zeta_1, \ldots, \zeta_n \rangle \in \mathbb{C}^n$, the integral

$$\hat{f}(\zeta) = (2\pi)^{-n/2}\int e^{-i\zeta \cdot x} f(x)\, dx$$

is well defined. Furthermore, $\hat{f}(\zeta)$ is an entire analytic function of the n complex variables $\zeta_1, \zeta_2, \ldots, \zeta_n$ since we can differentiate under the

integral sign. In addition, if the support of f is contained in the sphere of radius R, then an integration by parts yields

$$\prod_{i=1}^{n}(i\zeta_i)^{\alpha_i}\hat{f}(\zeta) = (2\pi)^{-n/2}\int_{|x|\le R} e^{-i\zeta\cdot x}D^{\alpha}f(x)\,dx$$

Taking the absolute value of both sides and using the fact that $\hat{f}(\zeta)$ is bounded on the set $\{\zeta \mid |\operatorname{Im}\zeta| < \varepsilon\}$, we easily conclude that for each N,

$$|\hat{f}(\zeta)| \le \frac{C_N e^{R|\operatorname{Im}\zeta|}}{(1+|\zeta|)^N} \qquad \text{for all } \zeta \in \mathbb{C}^n$$

where C_N is a constant that depends on N and f. The interesting fact is that these estimates are not only necessary but also sufficient for f to be in $C_0^{\infty}(\mathbb{R}^n)$.

Theorem IX.11 (the Paley–Wiener theorem) An entire analytic function of n complex variables $g(\zeta)$ is the Fourier transform of a $C_0^{\infty}(\mathbb{R}^n)$ function with support in the ball $\{x \mid |x| \le R\}$ if and only if for each N there is a C_N so that

$$|g(\zeta)| \le \frac{C_N e^{R|\operatorname{Im}\zeta|}}{(1+|\zeta|)^N} \tag{IX.6}$$

for all $\zeta \in \mathbb{C}^n$.

Proof We have already proven the "only if" part. Suppose that g is entire and satisfies estimates of the form (IX.6). Let $\zeta = \lambda + i\eta$, where $\lambda, \eta \in \mathbb{R}^n$. Then for each η, $g(\lambda + i\eta)$ is in $\mathcal{S}(\mathbb{R}^n)$ as a function of λ, since the derivatives fall off polynomially by (IX.6) and the Cauchy formula. Let

$$f(x) = (2\pi)^{-n/2}\int_{\mathbb{R}^n} e^{ix\cdot\lambda}g(\lambda)\,d\lambda \tag{IX.7}$$

Then by Theorem IX.1, $f \in \mathcal{S}(\mathbb{R}^n)$ and $g(\lambda) = \hat{f}(\lambda)$. We want to show that $f(x)$ has support in the ball of radius R. Because of the estimates (IX.6) and Cauchy's theorem, we can shift the region of integration in (IX.7) so that

$$f(x) = (2\pi)^{-n/2}\int_{\mathbb{R}^n} e^{i(\lambda+i\eta)\cdot x}g(\lambda+i\eta)\,d\lambda \tag{IX.8}$$

Thus, by (IX.6)

$$|f(x)| \le e^{R|\eta|-x\cdot\eta}(2\pi)^{-n/2}\int \frac{C_N}{(1+|\lambda+i\eta|)^N}\,d\lambda$$

$$\le e^{R|\eta|-x\cdot\eta}(2\pi)^{-n/2}\int \frac{C_N}{(1+|\lambda|)^N}\,d\lambda$$

where we have chosen N large enough so that the integral on the right is finite. Now, $f(x)$ does not depend on η, so if we let $\eta \to \infty$ in an appropriate direction, we conclude that $|f(x)| = 0$ if $|x| > R$. ∎

This theorem has a natural generalization to the distributions with compact support. Recall that a distribution $T \in \mathscr{S}'(\mathbb{R}^n)$ has support in a closed set K if and only if $T(\varphi) = 0$ for every test function φ with support in $\mathbb{R}^n \backslash K$. If K is compact, then T is said to have **compact support**. The set of distributions with compact support is the dual space of $\mathscr{E}(\mathbb{R}^n)$ (see Problems 39 and 40 of Chapter V).

Theorem IX.12 A distribution $T \in \mathscr{S}'(\mathbb{R}^n)$ has compact support if and only if $\hat{T}$ has an analytic continuation to an entire analytic function of n variables $\hat{T}(\zeta)$ that satisfies

$$|\hat{T}(\zeta)| \leq C(1 + |\zeta|)^N e^{R|\operatorname{Im}\zeta|} \tag{IX.9}$$

for all $\zeta \in \mathbb{C}^n$ and some constants C, N, R. Moreover, if (IX.9) holds, the support of T is contained in the ball of radius R.

Proof Suppose that $T \in \mathscr{S}'(\mathbb{R}^n)$ has compact support and let φ be a $C_0^\infty(\mathbb{R}^n)$ function which is equal to one on the support of T. Define $F(\zeta) = T[(2\pi)^{-n/2} e^{-i\zeta \cdot x}\varphi(x)]$. By Theorem IX.5, $F(\lambda + i0)$ is the Fourier transform of T. Furthermore, since

$$\left(\frac{\exp(-i(x_j(\zeta_j + h_j) + \sum_{k \neq j} \zeta_k x_k))\varphi(x) - e^{-i\zeta \cdot x}\varphi(x)}{h_j}\right)$$

$$\xrightarrow{\mathscr{S}(\mathbb{R}^n)} -ix_j e^{-i\zeta \cdot x}\varphi(x)$$

and $T \in \mathscr{S}'(\mathbb{R}^n)$, $F(\zeta)$ is differentiable in the complex sense in each variable and is thus entire.

Since $T \in \mathscr{S}'(\mathbb{R}^n)$,

$$|T(f)| \leq C_1 \sum_{\substack{|\alpha| \leq N \\ |\beta| \leq N}} \|x^\alpha D^\beta f\|_\infty$$

for some N and C_1 and all $f \in \mathscr{S}(\mathbb{R}^n)$. Thus, if φ has support in the sphere of radius R, then

$$|F(\zeta)| \leq C_2(1 + R^n)(1 + |\zeta|^N)e^{|\operatorname{Im}\zeta|R}$$

Conversely, suppose that $F(\zeta)$ is an entire function satisfying the estimate (IX.9). Then $F(\lambda + i0) \in \mathscr{S}'(\mathbb{R}^n)$, so it is the Fourier transform of some $T \in \mathscr{S}'(\mathbb{R}^n)$. Let $j_\varepsilon(x)$ be an approximate identity. Then by Theorem IX.4,

$\widehat{T * j_\varepsilon} = (2\pi)^{-n/2}\hat{j}_\varepsilon(\lambda)F(\lambda)$. Since j_ε has compact support in $\{x \mid |x| \leq \varepsilon\}$, we know by the Paley–Wiener theorem, that for each M we can find a constant C_M so that

$$|\hat{j}_\varepsilon(\zeta)| \leq \frac{C_M}{(1 + |\zeta|)^{N+M}} e^{\varepsilon|\operatorname{Im}\zeta|}$$

Therefore

$$|(2\pi)^{-n/2}\hat{j}_\varepsilon(\zeta)F(\zeta)| \leq \frac{C_M C e^{(R+\varepsilon)|\operatorname{Im}\zeta|}}{(1 + |\zeta|)^N}$$

which implies (again by the Paley–Wiener theorem) that the support of $T * j_\varepsilon$ is contained in the sphere of radius $R + \varepsilon$. Since ε is arbitrary and $(T * j_\varepsilon) \to T$ weakly, we conclude that the support of T is contained in the sphere of radius R about the origin. ∎

One natural way to extend the above theorems is to replace "compact support" with some weaker notion of decay at infinity. The following pair of theorems (whose proofs are outlined in Problem 76) will be used in Chapter XIII to prove the exponential decay of bound states of atomic Hamiltonians.

Theorem IX.13 Let f be in $L^2(\mathbb{R}^n)$. Then $e^{b|x|}f \in L^2(\mathbb{R}^n)$ for all $b < a$ if and only if $\hat{f}$ has an analytic continuation to the set $\{\zeta \mid |\operatorname{Im}\zeta| < a\}$ with the property that for each $\eta \in \mathbb{R}^n$ with $|\eta| < a$, $\hat{f}(\cdot + i\eta) \in L^2(\mathbb{R}^n)$ and for any $b < a$

$$\sup_{|\eta| \leq b} \|\hat{f}(\cdot + i\eta)\|_2 < \infty$$

Theorem IX.14 Let T be in $\mathscr{S}'(\mathbb{R}^n)$. Suppose that $\hat{T}$ is a function with an analytic continuation to the set $\{\zeta \mid |\operatorname{Im}\zeta| < a\}$ for some $a > 0$. Suppose further that for each $\eta \in \mathbb{R}^n$ with $|\eta| < a$, $\hat{T}(\cdot + i\eta) \in L^1(\mathbb{R}^n)$ and for any $b < a$, $\sup_{|\eta| < b} \|\hat{T}(\cdot + i\eta)\|_1 < \infty$. Then T is a bounded continuous function and for any $b < a$, there is a constant C_b so that

$$|T(x)| \leq C_b e^{-b|x|}$$

The next natural question to ask is what are the analyticity properties of a function or distribution with support on a half-line, half-space, or in general in a cone? As a simple example, consider the Fourier transform $\hat{f}$ of

a function $f \in \mathscr{S}(\mathbb{R})$ which has support contained in $[0, \infty)$. The reader can easily verify that

$$\hat{f}(\lambda - i\eta) = (2\pi)^{-1/2} \int e^{-i(\lambda - i\eta)\cdot x} f(x)\, dx \tag{IX.10}$$

is a well-defined analytic function in the open lower half-plane (i.e. for $\eta > 0$) and that $\hat{f}(\cdot - i\eta) \xrightarrow{\mathscr{S}(\mathbb{R})} \hat{f}$ as $\eta \downarrow 0$. That is, $\hat{f}$, which need not be real analytic, is the "boundary value" of an analytic function in the lower half-plane. The study of the Fourier transforms of functions and distributions with supports in half-spaces dates back to the classical investigations of the Laplace transform and has played an important role in modern analysis. The main ideas and techniques are similar to those used above in Theorem IX.11 and Theorem IX.12. However, an additional difficulty arises since one must specify in what sense the Fourier transform is the "boundary value" of the analytic function. There is a wide range of such theorems; we will discuss one which we will use in Section IX.8 in our study of quantum field theory. Some of the others are briefly discussed in the Notes.

Definition Let $a \in \mathbb{R}^n$, $|a| = 1$, and $\theta \in (0, \pi/2)$. Then

$$\Gamma_{a,\theta} = \{\xi \in \mathbb{R}^n \mid \xi \cdot a > |\xi| \cos\theta\}$$

is called the **cone about a of opening angle θ**. The cone $\Gamma^*_{a,\theta} \equiv \Gamma_{a,\pi/2-\theta}$ is called the **dual cone**. When no confusion arises, we will drop the subscripts and just refer to Γ and Γ^*.

The dual cone Γ^* will either contain Γ (as in Figure IX.1) or be contained in Γ. Notice that Γ^* is the interior of the intersection of the half-spaces $\{\eta \mid \eta \cdot \xi > 0\}$ for $\xi \in \Gamma$. If Γ is the open forward light cone in $\mathbb{R}^4$ (with the velocity of light equal to one), then Γ^* is also the open forward light cone. Given an open cone $C \subset \mathbb{R}^n$, we will denote by $\mathbb{R}^n - iC$ the open region of those $\zeta = \langle \lambda_1 - i\eta_1, \lambda_2 - i\eta_2, \ldots, \lambda_n - i\eta_n \rangle \in \mathbb{C}^n$ so that $\lambda = \langle \lambda_1, \ldots, \lambda_n \rangle \in \mathbb{R}^n$ and $\eta = \langle \eta_1, \ldots, \eta_n \rangle \in C$. $\mathbb{R}^n - iC$ is called the **tube with base C**.

We can now say what we mean by "boundary value."

Definition Let $S \in \mathscr{S}'(\mathbb{R}^n)$ and suppose $F(\zeta)$ is a function analytic in $\mathbb{R}^n - iC$ for some cone C. Suppose that for each fixed $\eta_0 \in C$, $F(\lambda - i\eta_0)$ is a tempered distribution (i.e. has at most polynominal growth in λ) and that as $t \downarrow 0$ in $\mathbb{R}$

$$\int_{\mathbb{R}^n} F(\lambda - it\eta_0)\varphi(\lambda)\, d\lambda \to S(\varphi)$$

for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$. Then S is said to be the (distributional) **boundary value of F in the sense of $\mathscr{S}'(\mathbb{R}^n)$**.

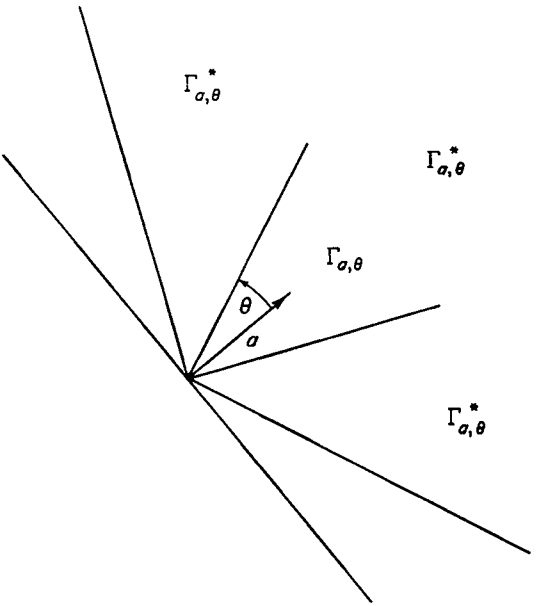


FIGURE IX.1 The cones $\Gamma_{a,\theta}$ and $\Gamma^*_{a,\theta}$.

Suppose that $T \in \mathscr{S}'(\mathbb{R}^n)$ and that the support of T is contained in $\overline{\Gamma}_{a,\theta}$ for some $a \in \mathbb{R}^n$ and $\theta \in (0, \pi/2)$. If T is given by a function $T(x)$, then we can directly extend $\hat{T}$ to the tube $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ by

$$\hat{T}(\lambda - i\eta) = (2\pi)^{-n/2} \int_{\Gamma_{a,\theta}} e^{-i(\lambda - i\eta)\cdot x} T(x)\, dx$$

For $\eta \in \Gamma^*_{a,\theta}$, the integral makes sense since

$$|e^{-i(\lambda - i\eta)\cdot x}| = e^{-|\eta||x|\cos(\eta, x)} \leq e^{-|x|\, d(\eta)}$$

where $d(\eta) \equiv |\eta| \min_{x \in \partial\Gamma_{a,\theta}} \cos(\eta, x) = \operatorname{dist}(\eta, \partial\overline{\Gamma}^*_{a,\theta})$; see Figure IX.1. Since $T(x)$ is polynomially bounded, the presence of the factor $e^{-|x|\, d(\eta)}$ means that we may differentiate under the integral sign. We conclude that $\hat{T}(\lambda - i\eta)$ is analytic in the tube $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ since it is infinitely differentiable in the complex sense. Furthermore, if $\varphi \in \mathscr{S}(\mathbb{R}^n)$, and $\eta_0 \in \Gamma^*_{a,\theta}$, then

$$\int_{\mathbb{R}^n} \hat{T}(\lambda - it\eta_0)\varphi(\lambda)\, d\lambda = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \int_{\Gamma_{a,\theta}} e^{-i(\lambda - it\eta_0)\cdot x} \varphi(\lambda) T(x)\, dx\, d\lambda$$

$$= \int_{\Gamma_{a,\theta}} e^{-t\eta_0 \cdot x} \hat{\varphi}(x) T(x)\, dx$$

$$\xrightarrow{t \downarrow 0} \int_{\Gamma_{a,\theta}} \hat{\varphi}(x) T(x)\, dx = \hat{T}(\varphi)$$

by the dominated convergence theorem. Thus, $\hat{T}$ is the boundary value of $\hat{T}(\lambda - i\eta)$ in the tube $\mathbb{R}^n - i\Gamma^*_{a,\theta}$.

If T is not a function but is of the form $P(D)G$ where G is a polynomially bounded continuous function with support in $\Gamma_{a,\theta}$, then we can define

$$\hat{T}(\lambda - i\eta) = (2\pi)^{-n/2} P(i(\lambda - i\eta)) \int_{\Gamma_{a,\theta}} e^{-i(\lambda - i\eta)\cdot x} G(x)\, dx$$

In the same way as above, one can then show that $\hat{T}(\lambda - i\eta)$ is analytic in $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ and that $\hat{T}$ is the boundary value of $\hat{T}(\lambda - i\eta)$. Thus, we wish to prove that *every* tempered distribution T with support in a cone can be written $T = P(D)G$ for some partial differential operator $P(D)$ and some polynomially bounded continuous function G *with support in the cone.* To see that this is a strong statement the reader should recall that the analogous statement for compact sets (rather than cones) is false. For example, the delta function cannot be written as $P(D)G$ where G has support at the origin.

Theorem IX.15 (Bros–Epstein–Glaser lemma) Let Γ be a proper open convex cone in $\mathbb{R}^n$ and let $T \in \mathscr{S}'(\mathbb{R}^n)$ have support in Γ. Then there exists a polynomially bounded continuous function G *with support in* Γ and a partial differential operator $P(D)$ so that $T = P(D)G$.

Proof Let $\{\mathbf{e}_i\}_{i=1}^n$ be a basis for $\mathbb{R}^n$ consisting of vectors in Γ. Every vector $x \in \mathbb{R}^n$ may be uniquely written $x = \sum_{i=1}^n y_i \mathbf{e}_i$ so that we may use $\{y_i\}_{i=1}^n$ as coordinates for $\mathbb{R}^n$. Define

$$F_m(y_1, \ldots, y_n) = (m!)^{-n} y_1^m y_2^m \cdots y_n^m \theta(y_1) \cdots \theta(y_n)$$

where θ is the characteristic function of $\{x \mid x \in \mathbb{R},\ x \geq 0\}$. Then $F_m \in C^{m-1}(\mathbb{R}^n)$ and F_m has support in Γ. Furthermore, if $Q(D) = \partial^n/\partial y_1 \cdots \partial y_n$, then $Q(D)^{m+1} F_m = \delta$ as the reader can easily check. We will show that for m sufficiently large, the convolution $T * F_m$ is a well-defined continuous function with support in Γ and that $Q(D)^{m+1}(T * F_m) = T * Q(D)^{m+1} F_m = T * \delta = T$.

If $b \in \Gamma$, then Γ is contained in the interior of $\Gamma - b$ so we may find a C^∞ function ψ that equals one on Γ and has support in $\Gamma - b$ (see Figure IX.2). Since $T \in \mathscr{S}'(\mathbb{R}^n)$, there is an N so that

$$|T(\varphi)| = |T(\psi\varphi)| \leq C_1 \sum_{\substack{|\alpha| \leq N \\ |\beta| \leq N}} \|x^\alpha D^\beta(\psi\varphi)\|_\infty$$

$$\leq C_2 \sum_{\substack{|\alpha| \leq N \\ |\alpha| \leq N}} \left(\sup_{x \in \bar{\Gamma} - b} |x^\alpha D^\beta \varphi(x)| \right) \equiv |||\varphi|||_b$$

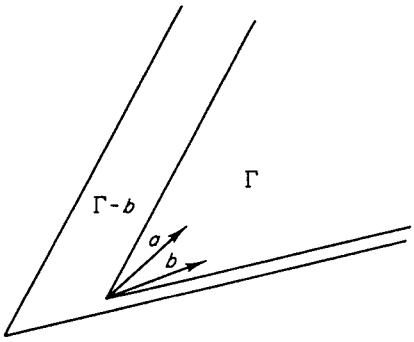


FIGURE IX.2 The cone $\Gamma - b$.

Thus, T has a unique extension, continuous in $|||\cdot|||_b$, to those C^N functions f for which $(\text{supp } f) \cap (\overline{\Gamma} - b)$ is compact.

Choose $m = N + 1$ and for $y \in \mathbb{R}^n$ define $\tilde{F}_{N+1;\,y}(x) = F_{N+1}(y - x)$. Then $\tilde{F}_{N+1;\,y}$ is a C^N function and $(\text{supp } \tilde{F}_{N+1;\,y}) \cap \overline{\Gamma} - b$ is compact (see Figure IX.3). Further, the map $y \to \tilde{F}_{N+1;\,y}$ is $|||\cdot|||_b$-continuous and polynomially bounded in y (see Figure IX.2). Thus, $G(y) = T * F_{N+1}(y) \equiv T(\tilde{F}_{N+1;\,y})$ is a polynomially bounded continuous function and supp $G \subset \overline{\Gamma}$ since

$$(\text{supp } \tilde{F}_{N+1;\,y}) \cap \overline{\Gamma} = \varnothing \qquad \text{if } y \notin \overline{\Gamma}$$

Furthermore, if $f \in C_0^\infty(\mathbb{R}^n)$, then

$$(f * G)(y) = T((f * F_{N+1})\tilde{}_y) \tag{IX.11}$$

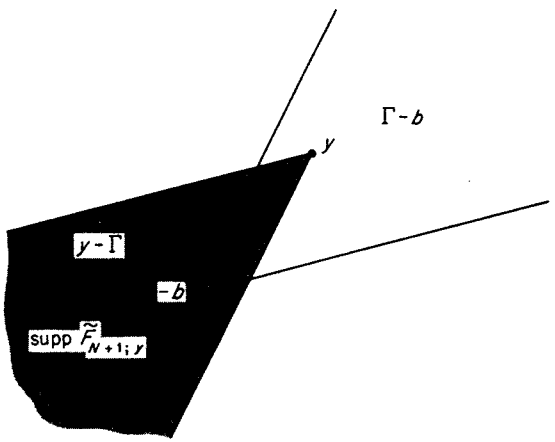


FIGURE IX.3 The support of $F_{N+1;\,y}$.

and

$$D^{\alpha}(f * G)(y) = T((D^{\alpha}f * F_{N+1})\tilde{}_{y}) \tag{IX.12}$$

These formulas are analogous to those in Theorem IX.4. Both may be proven by writing approximate Riemann sums for the integrals on the right and then observing that the approximate Riemann sums converge in $|||\cdot|||_b$. If we now let $j_\varepsilon(x)$ be an approximate identity, then by the proposition at the end of Section IX.1,

$$Q(D)^{N+2}G = \lim_{\varepsilon \downarrow 0} Q(D)^{N+2}(j_\varepsilon * G)$$

[by (IX.12)]

$$= \lim_{\varepsilon \downarrow 0} T((Q(D)^{N+2}j_\varepsilon * F_{N+1})\tilde{}_{y})$$

(by Theorem IX.4)

$$= \lim_{\varepsilon \downarrow 0} T((j_\varepsilon * Q(D)^{N+2}F_{N+1})\tilde{}_{y})$$

$$= \lim_{\varepsilon \downarrow 0} T((\tilde{j}_\varepsilon)_y)$$

$$= \lim_{\varepsilon \downarrow 0} j_\varepsilon * T = T \blacksquare$$

Theorem IX.16 Let T be a tempered distribution with support in the cone $\Gamma_{a,\theta}$, $a \in \mathbb{R}^n$, $0 < \theta < \pi/2$. Then $\hat{T}$ is the boundary value in the sense of $\mathscr{S}'(\mathbb{R}^n)$ of a function $\hat{T}(\lambda - i\eta)$ analytic in the tube $\mathbb{R}^n - i\Gamma^*_{a,\theta}$. Moreover, $\hat{T}(\lambda - i\eta)$ satisfies the estimate

$$|\hat{T}(\lambda - i\eta)| \leq |P(\lambda - i\eta)|(1 + [\operatorname{dist}(\eta, \partial\Gamma^*_{a,\theta})]^{-N}) \tag{IX.13}$$

for a suitable polynomial P and positive integer N.

Conversely, suppose $F(\lambda - i\eta)$ is analytic in $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ and satisfies the weaker estimates:

(i) For each $\eta_0 \in \Gamma^*_{a,\theta}$, there is a polynomial P_{η_0} in $2n$ variables so that

$$|F(\lambda - i(\eta_0 + \eta))| \leq |P_{\eta_0}(\lambda, \eta)|$$

for all $\lambda \in \mathbb{R}^n$ and $\eta \in \Gamma^*_{a,\theta}$.

(ii) There is an integer $r \geq 0$ so that for each $\eta_0 \in \Gamma^*_{a,\theta}$, there is a polynomial Q_{η_0} so that

$$|F(\lambda - it\eta_0)| \leq \frac{|Q_{\eta_0}(\lambda)|}{t^r}$$

for all $\lambda \in \mathbb{R}^n$ and $t \in (0, 1]$.

Then there is a tempered distribution T with support in the cone $\overline{\Gamma}_{a,\theta}$ so that $\hat{T}$ is the boundary value of $F(\lambda - i\eta)$ in the sense of $\mathscr{S}'(\mathbb{R}^n)$. Moreover, F can be recovered from T by the formula

$$F(\cdot - i\eta) = \widehat{e^{-\eta \cdot x} T} \tag{IX.14}$$

Proof Suppose that $T \in \mathscr{S}'(\mathbb{R}^n)$ and supp $T \subset \overline{\Gamma}_{a,\theta}$. By the Bros–Epstein–Glaser lemma, there is a polynomially bounded continuous function G with support in $\overline{\Gamma}_{a,\theta}$ so that $T = P(D)G$ for some partial differential operator $P(D)$. From the discussion before the lemma, we already know that $\hat{T}$ is the boundary value of the function

$$\hat{T}(\lambda - i\eta) = (2\pi)^{-n/2} P(i(\lambda - i\eta)) \int_{\mathbb{R}^n} e^{-i(\lambda - i\eta)\cdot x} G(x)\, dx$$

Thus,

$$|\hat{T}(\lambda - i\eta)| \leq (2\pi)^{-n/2} |P(i(\lambda - i\eta))| \int_{\mathbb{R}^n} e^{-|x|\, d(\eta)} |G(x)|\, dx$$

$$\leq C |P(i(\lambda - i\eta))| (1 + (d(\eta))^{-N})$$

since $G(x)$ has support in $\overline{\Gamma}_{a,\theta}$ and grows no worse at ∞ than $|x|^{N-n}$ for some N. This completes the proof in the first direction.

Conversely, we suppose that $F(\lambda - i\eta)$ is analytic in $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ and that the estimates (i) and (ii) hold. The proof is in several steps. First we show that $F(\lambda - it\eta)$ has a tempered distribution $\hat{T}_\eta$ as boundary value as $t \downarrow 0$. Then we show that the limit is independent of η. Finally we show that T has support in $\overline{\Gamma}_{a,\theta}$.

For each fixed $\eta_0 \in \Gamma^*_{a,\theta}$, $0 < t \leq 1$, $F(\lambda - it\eta_0)$ is a well-defined distribution in $\mathscr{S}'(\mathbb{R}^n)$ which we denote by $\hat{T}_{t,\eta_0}$. Let $\psi \in \mathscr{S}(\mathbb{R}^n)$ and set

$$h(t) = \int_{\mathbb{R}^n} F(\lambda - it\eta_0)\psi(\lambda)\, d\lambda = \hat{T}_{t,\eta_0}(\psi)$$

Then,

$$\frac{d^j}{dt^j} h(t) = \int_{\mathbb{R}^n} F(\lambda - it\eta_0) \left(i\eta_0 \cdot \frac{\partial}{\partial \lambda} \right)^j \psi(\lambda)\, d\lambda$$

so,

$$\left|\frac{d^j}{dt^j}h(t)\right| \leq C \sup_{\lambda} \frac{|Q_{\eta_0}(\lambda)(1+|\lambda|)^k||(i\eta_0\cdot\partial/\partial\lambda)^j\psi(\lambda)|}{t^r} \tag{IX.15}$$

where k has been chosen large enough so that $\int_{\mathbb{R}^n}(1+|\lambda|)^{-k}\,d\lambda$ converges.

Let $p = r + 2$. Then, by the fundamental theorem of calculus,

$$h(t_1) = -\int_{t_1}^{1}\int_{t_2}^{1}\cdots\int_{t_{p-1}}^{1}\left(\frac{d^p}{dt^p}h(t_p)\right)dt_p\cdots dt_2 + h(1) + \sum_{j=1}^{p-1}Q_j(t_1)\left(\frac{d^j}{dt_1^j}h\right)(1)$$

where the Q_j are suitable polynomials. The estimates (IX.15) show that the limit of $h(t_1)$ exists as $t_1 \downarrow 0$ and that each term in the limit is less than or equal to a constant times an $\mathscr{S}(\mathbb{R}^n)$-seminorm of ψ. Thus $F(\lambda - it\eta_0)$ converges in $\mathscr{S}'(\mathbb{R}^n)$ as $t \downarrow 0$ to a tempered distribution which we will denote by $\hat{T}_{0,\eta_0}$. Now suppose that $\eta_1, \eta_2 \in \Gamma^*_{a,\theta}$ and that $\check{\psi}(x)$ is in $C_0^\infty(\mathbb{R}^n)$. Then

$$\begin{aligned}\hat{T}_{t,\eta_1}(\psi) &= \int_{\mathbb{R}^n} F(\lambda - it\eta_2 + it(\eta_2 - \eta_1))\psi(\lambda)\,d\lambda \\ &= \int_{\mathbb{R}^n} F(\lambda - it\eta_2)\psi(\lambda - it(\eta_2 - \eta_1))\,d\lambda \\ &= T_{t,\eta_2}(\widehat{e^{-t(\eta_2-\eta_1)\cdot x}\check{\psi}(x)})\end{aligned}$$

where we have used the fact that $\psi(\lambda)$ is entire and the estimates on $\psi(\lambda)$ in the Paley–Wiener theorem to shift the hyperplane of integration in the second step. Since $\check{\psi} \in C_0^\infty(\mathbb{R}^n)$, $\widehat{e^{-t(\eta_2-\eta_1)\cdot x}\check{\psi}(x)} \xrightarrow{\mathscr{S}(\mathbb{R}^n)} \psi$ as $t \downarrow 0$. Thus by Theorem V.8,

$$\hat{T}_{t,\eta_2}(e^{-t(\eta_2-\eta_1)\cdot x}\check{\psi}(x)) \to \hat{T}_{0,\eta_2}(\psi)$$

and therefore $\hat{T}_{0,\eta_1}(\psi) = \hat{T}_{0,\eta_2}(\psi)$. Since such ψ are dense in $\mathscr{S}(\mathbb{R}^n)$, $\hat{T}_{0,\eta_1} = \hat{T}_{0,\eta_2}$. Thus, the limit of $\hat{T}_{t,\eta_0}$ as $t \downarrow 0$ is independent of η_0; we denote the limit by $\hat{T}$.

We have shown that $F(\lambda - i\eta)$ has a tempered distribution $\hat{T}$ as a boundary value. It remains to prove that its inverse Fourier transform T has support in $\Gamma_{a,\theta}$ and to verify (IX.14). Let $\eta_1 \in \Gamma^*_{a,\theta}$ be given and suppose that $\varphi \in C_0^\infty(\mathbb{R}^n)$ has compact support in the open half-space $\{x \mid \eta_1 \cdot x < 0\}$. Then there is $\varepsilon > 0$ so that $x \in \operatorname{supp}\varphi$ implies $\eta_1 \cdot x \leq -\varepsilon$.

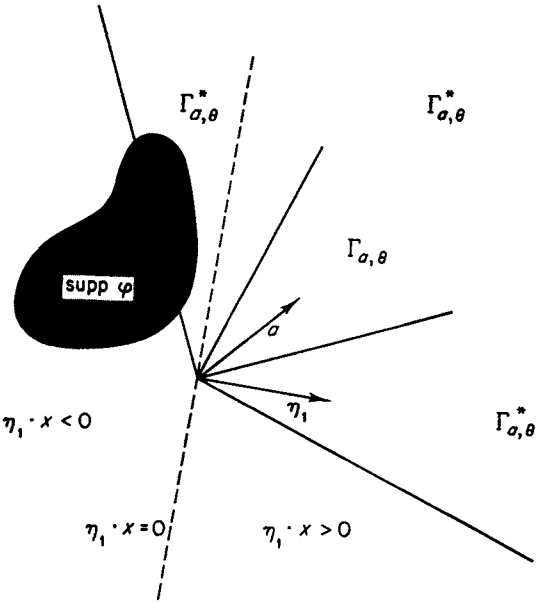


FIGURE IX.4 The support of φ.

See Figure IX.4. It follows that $\check{\varphi}$ is entire and that for each N

$$|\check{\varphi}(\lambda - is\eta_1)| = |(2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{i(\lambda - is\eta_1)\cdot x} \varphi(x)\, dx|$$

$$\leq \frac{C_N e^{-s\varepsilon}}{(1 + |\lambda - is\eta_1|^N)} \tag{IX.16}$$

for some constant C_N. Furthermore,

$$T_{t,\eta_1}(\varphi) = \hat{T}_{t,\eta_1}(\check{\varphi})$$

$$= \int F(\lambda - it\eta_1)\check{\varphi}(\lambda)\, d\lambda$$

$$= \int F(\lambda - i(t+s)\eta_1)\check{\varphi}(\lambda - is\eta_1)\, d\lambda$$

by Cauchy's formula. Thus, if we use the hypothesis (i) and choose N large enough in the estimate (IX.16), we find that for arbitrary $s > 0$,

$$|T_{t,\eta_1}(\varphi)| \leq Ce^{-s\varepsilon}$$

and thus $T_{t,\eta_1}(\varphi) = 0$. Therefore, the support of T_{t,η_1} is contained in the half-space $\{x \mid \eta_1 \cdot x \geq 0\}$ for each $t > 0$. Since $T_{t,\eta_1} \to T$ as $t \downarrow 0$, we conclude that supp $T \subset \{x \mid \eta_1 \cdot x \geq 0\}$. Since $\Gamma_{a,\theta}$ is the intersection of the closed subspaces $\{x \mid \eta_1 \cdot x \geq 0\}$ where η_1 runs through $\Gamma^*_{a,\theta}$, we see that supp $T \subset \Gamma_{a,\theta}$.

Finally, suppose $\check{\psi} \in C_0^\infty(\mathbb{R}^n)$ as above. Then

$$\begin{aligned}
\int_{\mathbb{R}^n} F(\lambda - i\eta)\psi(\lambda)\, d\lambda &= \int F(\tau - is\eta)\psi(\tau - (s-1)i\eta)\, d\tau \\
&= \hat{T}_{s,\eta}(\widehat{e^{-(s-1)\eta \cdot x}\check{\psi}}) \\
&\xrightarrow[s \to 0]{} \hat{T}(\widehat{e^{\eta \cdot x}\check{\psi}}) \\
&= T(e^{-\eta \cdot x}\hat{\psi}) \\
&= (e^{-\eta \cdot x}T)(\hat{\psi}) \\
&= (\widehat{e^{-\eta \cdot x}T})(\psi)
\end{aligned}$$

This proves (IX.4) and completes the proof of the theorem. ∎

We will use this theorem in our study of axiomatic quantum field theory in Section 9.

IX.4 L^p Estimates

There are a large number of L^p-estimates on Fourier transforms and convolutions. These estimates are useful because they give conditions on p and q so that the Fourier transform or convolution by a given function is a bounded map from L^p to L^q. The proofs of the estimates typically require delicate use of L^p-interpolation theorems. In this section we state several L^p-interpolation theorems and give examples to show how they may be used to derive estimates. In the Appendix, we prove the first of these theorems (Theorem IX.17) and use the idea of this proof to prove a variety of other interpolation theorems not used in this section.

The simplest L^p-interpolation theorem is:

Theorem IX.17 (The Riesz–Thorin theorem) Let $\langle M, \mu\rangle$ and $\langle N, \nu\rangle$ be measure spaces with σ-finite measures. Let $1 \leq p_0, p_1, q_0, q_1 \leq \infty$ and suppose that T is a linear transformation from $L^{p_0}(M, d\mu) \cap L^{p_1}(M, d\mu)$ to

$L^{q_0}(N, d\nu) \cap L^{q_1}(N, d\nu)$ which satisfies $\|Tf\|_{q_0} \le M_0\|f\|_{p_0}$ and $\|Tf\|_{q_1} \le M_1\|f\|_{p_1}$. Then, for each $f \in L^{p_0} \cap L^{p_1}$, and each $t \in (0, 1)$, $Tf \in L^{q_t}$ and $\|Tf\|_{q_t} \le C_t\|f\|_{p_t}$ where $p_t^{-1} = tp_1^{-1} + (1-t)p_0^{-1}$, $q_t^{-1} = tq_1^{-1} + (1-t)q_0^{-1}$, and $C_t = M_0^{1-t}M_1^t$.

Notice that if the hypotheses of the theorem are satisfied, then T can be extended by the B.L.T. theorem to be a bounded map from $L^{p_t}(M, d\mu)$ to $L^{q_t}(N, d\nu)$. The Riesz–Thorin theorem says essentially that the set of $\langle p^{-1}, q^{-1}\rangle$ so that T: $L^p(M, d\mu) \to L^q(N, d\nu)$ is bounded is a convex subset of the plane and that on that subset the logarithm of the norm of T is a convex function. The Riesz–Thorin theorem is a special case of the Stein interpolation theorem which is proven in the Appendix at the end of this section.

We have already given one application of this theorem in Section 2 (the Hausdorff–Young theorem). Here is another:

Example 1 (Young's theorem and inequality) When f and g are in $\mathscr{S}(\mathbb{R}^n)$ we defined the convolution by the formula

$$(f * g)(x) = \int f(x-y)g(y)\,dy \tag{IX.17}$$

Suppose $p^{-1} + q^{-1} = 1$. If $f \in L^p(\mathbb{R}^n)$ and $g \in L^q(\mathbb{R}^n)$, then the integral converges absolutely for all x by Hölder's inequality. Thus we can use (IX.17) to define $f * g$ when $f \in L^p$, $g \in L^q$. Note that $\|f * g\|_\infty \le \|f\|_p\|g\|_q$. Next, suppose that $f, g \in L^1(\mathbb{R}^n)$. Then

$$\iint |f(x-y)g(y)|\,dx\,dy = \|f\|_1\|g\|_1$$

so by Fubini's theorem the integral in (IX.17) exists a.e. in x, and the function $f * g$ (defined a.e.) satisfies $\|f * g\|_1 \le \|f\|_1\|g\|_1$. We can now use the Riesz–Thorin theorem to define the convolution on other L^p spaces.

Suppose that $f \in L^1(\mathbb{R}^n)$. Then $T_f(g) = f * g$ is a bounded operator from $L^1(\mathbb{R}^n)$ to $L^1(\mathbb{R}^n)$ (of norm less than or equal to $\|f\|_1$) and from $L^\infty(\mathbb{R}^n)$ to $L^\infty(\mathbb{R}^n)$ (of norm less than or equal to $\|f\|_1$). Therefore, by the Riesz–Thorin theorem, T_f: $L^p(\mathbb{R}^n) \to L^p(\mathbb{R}^n)$ and has norm less than or equal to $\|f\|_1$. Now fix $g \in L^p(\mathbb{R}^n)$. Then

$$\begin{aligned} &T_g\colon L^1(\mathbb{R}^n) \to L^p(\mathbb{R}^n), && \|T_g\| \le \|g\|_p \\ &T_g\colon L^q(\mathbb{R}^n) \to L^\infty(\mathbb{R}^n), && \|T_g\| \le \|g\|_p \end{aligned}$$

We now use the Riesz–Thorin theorem again to interpolate between 1 and q concluding that T_g: $L^r(\mathbb{R}^n) \to L^s(\mathbb{R}^n)$ with norm less than or equal to $\|g\|_p$ where $r^{-1} = 1 - tp^{-1}$ and $s^{-1} = (1-t)p^{-1}$. Eliminating t, we find that for $1 \le p, r, s, \le \infty$, satisfying $p^{-1} + r^{-1} = 1 + s^{-1}$,

$$\|f * g\|_s \le \|f\|_r \|g\|_p$$

This is known as Young's inequality.

It is sometimes important to know that the extended convolution from $L^p \times L^r$ to L^s which we have just defined by using the Riesz–Thorin theorem can still be computed a.e. by the integral formula (IX.17). The proof, like the extension, is in two stages. Let $p^{-1} + q^{-1} = 1$ and suppose that $f \in L^p$, $g \in L^1$, and $h \in L^q$. We may assume without loss that f, g, and h are positive. Then

$$\begin{aligned}\int h(x)\left(\int f(x-y)g(y)\,dy\right)dx &= \int g(y)\left(\int f(x-y)h(x)\,dx\right)dy \\ &\le \|f\|_p \|h\|_q \int g(y)\,dy \\ &= \|f\|_p \|h\|_q \|g\|_1\end{aligned}$$

Since this holds for all such h, the integral $\int f(x-y)g(y)\,dy$ converges a.e.[x] and is in L^p with norm less than or equal to $\|f\|_p\|g\|_1$. But the map $f \to \int f(x-y)g(y)\,dy$ agrees with the convolution for all $f \in L^1 \cap L^\infty$, so it agrees on all of L^p.

Now, we use the same trick again. Let $p^{-1} + r^{-1} = 1 + s^{-1}$ and suppose that $f \in L^p$, $g \in L^r$ and $h \in L^1 \cap L^{s'}$ where $s' = s(s-1)^{-1}$. Then, using the Hölder and Young inequalities we have

$$\begin{aligned}&\int g(y)\left(\int f(x-y)h(x)\,dx\right)dy \\ &\le \|g\|_r \|\tilde{f} * h\|_{r'} \\ &\le \|g\|_r \|\tilde{f}\|_p \|h\|_{s'}\end{aligned}$$

since by the first part of the argument the integral represents the convolution. Thus, by Fubini's theorem $g(y)f(x-y)h(x) \in L^1(\mathbb{R}^n \times \mathbb{R}^n)$, and as a function of y, $g(y)f(x-y)h(x) \in L^1(\mathbb{R}^n)$ for almost all x, and

$$\int h(x)\left(\int f(x-y)g(y)\,dy\right)dx \le \|g\|_r \|\tilde{f}\|_p \|h\|_{s'}$$

Since $h \in L^1 \cap L^{s'}$ was arbitrary, we conclude that $f(x-y)g(y) \in L^1(\mathbb{R}^n)$ as a function of y for almost all x and $\int f(x-y)g(y)\,dy \in L^s(\mathbb{R}^n)$ with norm less

than or equal to $\|f\|_p\|g\|_r$. Therefore, since the bounded maps $g \to f * g$ and $g \to \int f(x-y)g(y)\,dy$ agree on $L^1 \cap L^r$, they agree on L^r.

There is a classical result of Hardy and Littlewood which says that if $p^{-1} + q^{-1} + \lambda = 2$, $\lambda < 1$, and $p, q > 1$, then

$$\iint_{\mathbb{R}^2} |f(x)g(y)|\,|x-y|^{-\lambda}\,dx\,dy < \infty \tag{IX.18}$$

if $f \in L^p(\mathbb{R})$, $g \in L^q(\mathbb{R})$. This is a strengthening of Young's inequality, since Young's inequality can easily be transformed into the statement that if $p^{-1} + r^{-1} + q^{-1} = 2$, then

$$\left| \iint_{\mathbb{R}^2} f(x)g(y)h(x-y)\,dx\,dy \right| < \infty$$

if $f \in L^p(\mathbb{R})$, $g \in L^r(\mathbb{R})$, $h \in L^q(\mathbb{R})$. (IX.18) is a strengthening of this inequality since $|x|^{-1} \notin L^1(\mathbb{R})$ and therefore $|x|^{-\lambda} \notin L^{\lambda^{-1}}(\mathbb{R})$. In order to deal with situations like this it is useful to introduce classes of functions which are barely not in the L^p spaces.

Definition Let $\langle M, \mu \rangle$ be a measure space, μ a σ-finite measure. A function f on M is said to be in **weak-L^p**, written $f \in L^p_w(M, d\mu)$, if there is a constant $C < \infty$ so that

$$\mu\{x \mid |f(x)| > t\} \le Ct^{-p} \qquad \text{for all } t > 0$$

If $f \in L^p_w$, we write

$$\|f\|_{p,w} = \sup_t (t^p \mu\{x \mid |f(x)| > t\})^{1/p}$$

Notice that $\|\cdot\|_{p,w}$ is not a norm since it does not satisfy the triangle inequality. The name weak-L^p comes from the fact that $L^p \subset L^p_w$ and $\|f\|_{p,w} \le \|f\|_p$ (see Problem 24). Further, $f \in L^p$ if and only if

$$\int_0^\infty \mu\{x \mid |f(x)| > t\} t^{p-1}\,dt < \infty$$

This integral is at worst logarithmically divergent if $f \in L^p_w$.

Example 2 The function $|x|^{-n/p}$ from $\mathbb{R}^n$ to $\mathbb{R}$ has $\mu\{x \mid |f(x)| > t\} = c_n t^{-p}$ where c_n is the volume of the unit ball in $\mathbb{R}^n$. Thus f is in $L^p_w(\mathbb{R}^n, dx)$ but f is not in $L^q(\mathbb{R}^n, dx)$ for any q.

We state without proof two interpolation theorems about weak-L^p spaces. The proof of Hunt's theorem is outlined in the problems. References are given in the notes.

Theorem IX.18 (Marcinkiewicz interpolation theorem) Let $\langle M, \mu\rangle$ and $\langle N, \nu\rangle$ be σ-finite measure spaces and $1 \le p_0 \le q_0 \le \infty$, $1 \le p_1 \le q_1 \le \infty$, $q_0 \ne q_1$. Suppose that T is a linear transformation satisfying $T: L^{p_0}(M, d\mu) \to L^{q_0}_w(N, d\nu)$ and $T: L^{p_1}(M, d\mu) \to L^{q_1}_w(N, d\nu)$ with

$$\|T\varphi\|_{q_0, w} \le c_0\|\varphi\|_{p_0}$$
$$\|T\psi\|_{q_1, w} \le c_1\|\psi\|_{p_1}$$

for all $\varphi \in L^{p_0}(M, d\mu)$, $\psi \in L^{p_1}(M, d\mu)$. Then, for any $t \in (0, 1)$, T extends to a bounded linear transformation from $L^{p_t}(M, d\mu)$ to $L^{q_t}(N, d\nu)$ where $p_t^{-1} = tp_1^{-1} + (1-t)p_0^{-1}$ and $q_t^{-1} = tq_1^{-1} + (1-t)q_0^{-1}$. The bound depends only on t and the c_i, q_i, and p_i.

Theorem IX.19 (Hunt's interpolation theorem) Let $\langle M, \mu\rangle$ and $\langle N, \nu\rangle$ be σ-finite measure spaces and $1 \le p_1 < p_0 \le \infty$, $1 \le q_1 < q_0 \le \infty$. Suppose that T is a bounded linear transformation from $L^{p_0}(M, d\mu)$ to $L^{q_0}(N, d\nu)$ and from $L^{p_1}(M, d\mu)$ to $L^{q_1}(N, d\nu)$. Then for any $t \in (0, 1)$, T extends to a bounded linear map of $L^{p_t}(M, d\mu)$ to $L^{q_t}_w(N, d\nu)$ (p_t and q_t defined above). Moreover, $\|Tf\|_{q_t, w} \le C_t\|f\|_{p_t, w}$ where C_t depends only on t, p_i, q_i, and the bounds at the end points.

We remark that the Marcinkiewicz theorem is the deepest interpolation theorem since it turns "weak" information into strong information. The reader is cautioned to remember the $p < q$ condition (see Problem 77 for an example of the trouble that can be caused by forgetting it). Notice that we do not have the logarithmically convex bound in either of the "weak" theorems as we did in the Riesz–Thorin theorem.

As an application of how to use these theorems in tandem, we will prove a generalization of the Hardy–Littlewood inequality.

Example 3 (Sobolev's inequality) Let $0 < \lambda < n$ and suppose that $f \in L^p(\mathbb{R}^n)$, $h \in L^r(\mathbb{R}^n)$ with $p^{-1} + r^{-1} + \lambda n^{-1} = 2$ and $1 < p, r < \infty$. Then

$$\iint \frac{|f(x)|\,|h(y)|}{|x-y|^\lambda}\, d^n x\, d^n y \le C_{p,r,\lambda,n}\|f\|_p\|h\|_r \tag{IX.19}$$

To prove this we need the following extension of Young's inequality: If $1 < p, r, s < \infty$, $p^{-1} + r^{-1} = s^{-1} + 1$, $f \in L^p(\mathbb{R}^n)$, $g \in L^r_w(\mathbb{R}^n)$, then

$f * g \in L^s(R^n)$ and $\|f * g\|_s \leq C\|f\|_p\|g\|_{r,w}$. First fix $f \in L^p(\mathbb{R}^n)$. Then Young's inequality (Example 1) shows that T_f: $L^r(\mathbb{R}^n) \to L^s(\mathbb{R}^n)$ where $T_f(g) = f * g$ and $1 \leq r \leq p'$. Choosing first $r = 1$ and then $r = p'$ and using Hunt's theorem we conclude that for $1 < r < p'$, T_f: $L^r_w(\mathbb{R}^n \to L^s_w(\mathbb{R}^n)$ is bounded. Now, we fix $g \in L^r_w(\mathbb{R}^n)$. We know that T_g: $L^p(\mathbb{R}^n) \to L^s_w(\mathbb{R}^n)$ is bounded for p and s suitably related and $p \leq s$. Using the Marcinkiewicz theorem we conclude that $f * g \in L^s(\mathbb{R}^n)$. Sobolev's inequality follows directly from this extended version of Young's inequality.

Table IX.1 summarizes some of the most important L^p inequalities on $\mathbb{R}^n$. There are also L^p estimates involving derivatives which we discuss in the Notes to Section IX.6.

TABLE IX.1

Name	Conditions	Inequality
Hölder	$1 \leq p, q, r \leq \infty$ $p^{-1} + q^{-1} = r^{-1}$	$\|fg\|_r \leq \|f\|_p\|g\|_q$
Hausdorff–Young	$1 \leq p \leq 2$ $p^{-1} + q^{-1} = 1$	$\|\hat{f}\|_q \leq (2\pi)^{(n/2-n/p)}\|f\|_p$
Young	$1 \leq p, q, r \leq \infty$ $p^{-1} + q^{-1} = 1 + r^{-1}$	$\|f * g\|_r \leq \|f\|_p\|g\|_q$
Generalized Young	$1 < p, q, r < \infty$ $p^{-1} + q^{-1} = 1 + r^{-1}$	$\|f * g\|_r \leq C_{p,q}\|f\|_p\|g\|_{q,w}$
Weak Hausdorff–Young	$1 < p < 2$ $p^{-1} + q^{-1} = 1$	$\|\hat{f}\|_{q,w} \leq C_{p,n}\|f\|_{p,w}$
Weak Young	$1 < r, p, s < \infty$ $p^{-1} + q^{-1} = 1 + r^{-1}$	$\|f * g\|_{r,w} \leq C_{p,q}\|f\|_{p,w}\|g\|_{q,w}$

Appendix to IX.4 Abstract interpolation

In this appendix, we prove an abstract interpolation theorem and then give several applications including a proof of the Stein and Riesz–Thorin theorems. Before turning to the abstract theory we present two propositions which illustrate the basic idea behind interpolation.

Proposition 1 Let A and B be matrices on the inner product space $\mathbb{C}^n$ with $A \geq 0$. Suppose that $\|AB\| \leq 1$ and $\|BA\| \leq 1$. Then $\|A^{1/2}BA^{1/2}\| \leq 1$.

Proof Suppose that Proposition 1 is true for all $A > 0$. Then we can prove the proposition for all $A \geq 0$ as follows. Given $A \geq 0$ and the conditions $\|AB\| \leq 1$, $\|BA\| \leq 1$, let $c > 0$ and define $B' = B(1 + c\|B\|)^{-1}$. Then $\|(A + c)B'\| \leq 1$ and $\|B'(A + c)\| \leq 1$. Since $A + c > 0$ we conclude that $\|(A + c)^{1/2}B'(A + c)^{1/2}\| \leq 1$. Letting $c \downarrow 0$ we conclude that

$$\|A^{1/2}BA^{1/2}\| \leq 1$$

Thus we may assume that $A > 0$.

How shall we turn information about AB and BA into information about $A^{1/2}BA^{1/2}$? Since A^x is a well-defined self-adjoint operator, it is natural to introduce the function $F(x) = A^xBA^{1-x}$. We then notice that $F(x)$ has an analytic continuation, $F(z) = A^zBA^{1-z} = e^{z \log A}Be^{(1-z)\log A}$ to the entire complex plane. Thus, the hypotheses of Proposition 1 tell us that the particular matrix-valued analytic function $F(z)$ has the properties $\|F(0)\| \leq 1$ and $\|F(1)\| \leq 1$. We must use these inequalities to conclude that $\|F(\frac{1}{2})\| \leq 1$. To do this we use a classical result in function theory due to Hadamard:

Lemma (Hadamard's three line theorem) Let $\varphi(z)$ be a complex-valued function, bounded and continuous on the closed strip $\{z \mid 0 \leq \operatorname{Re} z \leq 1\}$, analytic in the interior, satisfying

$$|\varphi(z)| \leq M_0 \qquad \text{if} \quad \operatorname{Re} z = 0$$

and

$$|\varphi(z)| \leq M_1 \qquad \text{if} \quad \operatorname{Re} z = 1$$

Then $|\varphi(z)| \leq M_0^{1-\operatorname{Re} z}M_1^{\operatorname{Re} z}$ for all z in the strip.

Proof We may take $M_0 = 1 = M_1$ since we can always replace $\varphi(z)$ by $\varphi(z)M_0^{z-1}M_1^{-z}$. We must show that $|\varphi(z)| \leq 1$ in the strip. If $\varphi(z) \to 0$ at ∞ in the strip, then $|\varphi(z)| \leq 1$ by the maximum modulus principle. Otherwise, consider $\varphi_n(z) = \varphi(z)e^{z^2/n}e^{-1/n}$. Since $\varphi(z)$ is bounded, $\varphi_n(z) \to 0$ as $z \to \infty$ in the strip. Thus, $|\varphi_n(z)| \leq 1$ everywhere in the strip since $|\varphi_n| \leq 1$ on the boundary. This is true for all n, so $|\varphi(z)| \leq 1$ since $e^{z^2/n}e^{-1/n} \to 1$ as $n \to \infty$. ∎

Hadamard's theorem holds for Banach space-valued analytic functions by the same proofs. We will use this extended theorem without comment. We can now easily prove Proposition 1.

Conclusion of the proof of Proposition 1 If $y \in \mathbb{R}$, then $e^{iy \log A}$ is unitary, so $\|e^{iy \log A}\| = 1$. Thus, on the line $\operatorname{Re} z = 0$, we have $\|F(z)\| = \|BA\| \leq 1$ and on the line $\operatorname{Re} z = 1$, we have $\|F(z)\| = \|AB\| \leq 1$. Moreover, for $0 \leq \operatorname{Re} z \leq 1$, $\|F(z)\| \leq (1 + \|A\|)^2 \|B\|$. Thus, by the three line theorem, $\|F(z)\| \leq 1$ for all z in the strip $0 \leq \operatorname{Re} z \leq 1$. In particular, $\|F(\frac{1}{2})\| \leq 1$. ∎

The reader is invited to find a proof of Proposition 1 which does not use interpolation (Problem 51). The three line theorem also gives an easy proof of Holder's inequality:

Proposition 2 (Hölder's inequality) Let $\langle M, \mu \rangle$ be a measure space and suppose that $f \in L^p(M, d\mu)$ and $g \in L^q(M, d\mu)$ where $p^{-1} + q^{-1} = 1$. Then $fg \in L^1(M, d\mu)$ and $\|fg\|_1 \leq \|f\|_p \|g\|_q$.

Proof It is sufficient to prove Hölder's inequality in the case where f and g are nonnegative simple functions (finite linear combinations of characteristic functions of disjoint measurable sets of finite measure). Let

$$F(z) = \int_M f^{pz} g^{q(1-z)} \, d\mu$$

Then $F(z)$ is continuous and bounded on the strip $0 \leq \operatorname{Re} z \leq 1$ and analytic in the interior. If $\operatorname{Re} z = 0$, then

$$|F(z)| \leq \int |f^{pz} g^{q(1-z)}| \, d\mu = \int |g|^q \, d\mu = \|g\|_q^q$$

and if $\operatorname{Re} z = 1$,

$$|F(z)| \leq \int |f^{pz} g^{q(1-z)}| \, d\mu = \int |f|^p \, d\mu = \|f\|_p^p$$

Thus, by the three line theorem $|F(x)| \leq \|g\|_q^{q(1-x)} \|f\|_p^{px}$ for all $0 \leq x \leq 1$. In particular for $x = p^{-1}$ we conclude that

$$F\left(\frac{1}{p}\right) = \int_M fg \, d\mu \leq \|g\|_q \|f\|_p \quad \blacksquare$$

The Hadamard theorem lies behind a general approach to interpolation theorems using complex methods (for other approaches, see the references in the Notes). Our discussion is divided into two parts. First we show that if X is a vector space with two norms $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ obeying a consistency condition, then it is possible to define a natural family of Banach spaces $\{X_t \mid 0 \leq t \leq 1\}$ which interpolate between X_0 and X_1, the completions of X in $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$. The abstract interpolation theorem

then follows easily; namely if $\{X_t\}$ interpolates between X_0 and X_1 and $\{Y_t\}$ interpolates between Y_0 and Y_1, then any map T which is in $\mathscr{L}(X_0, Y_0)$ and in $\mathscr{L}(X_1, Y_1)$ extends uniquely to a bounded map of X_t into Y_t for each t. In the second part we illustrate how the abstract theorem may be applied in specific cases. In particular, we will prove the Stein interpolation theorem, for which the Riesz-Thorin theorem is an immediate corollary, and several other interpolation theorems. The difficulty involved in the special cases is the concrete identification of the spaces $\{X_t\}$ and $\{Y_t\}$.

Definition Let X be a complex vector space. Two norms $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ on X are called **consistent** if any sequence $\{x_n\}$ that converges to zero in one norm and which is Cauchy in the other norm converges to zero in both norms. If $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ are consistent, we define

$$\|x\|_+ = \inf\{\|y\|^{(0)} + \|z\|^{(1)} \mid x = y + z\}$$

Proposition 3 Let $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ be consistent norms on a complex vector space X. Then:

(a) $\|\cdot\|_+$ is a norm.

(b) If X_0, X_1, and X_+ denote the completions of X under $\|\cdot\|^{(0)}$, $\|\cdot\|^{(1)}$, and $\|\cdot\|_+$, then the identity map on X extends to a continuous *injective* map of X_0 into X_+ and of X_1 into X_+.

Proof Suppose that $x \in X$ and $\|x\|_+ = 0$. Then there exist y_n and z_n such that $x = y_n + z_n$ and $y_n \xrightarrow{\|\cdot\|^{(0)}} 0$, $z_n \xrightarrow{\|\cdot\|^{(1)}} 0$. But then $y_n = x - z_n \xrightarrow{\|\cdot\|^{(1)}} x$, so $x = 0$ by the consistency of the norms. This proves (a).

Since $\|\cdot\|_+ \leq \|\cdot\|^{(0)}$, the identity map $\imath$ extends uniquely to a continuous map of X_0 into X_+. Suppose that $x \in X_0$ and $\imath(x) = 0$. Then, there exist $x_n \in X$ such that $x_n \xrightarrow{\|\cdot\|^{(0)}} x$ and $x_n \xrightarrow{\|\cdot\|_+} 0$. The second statement implies that there exist y_n, $z_n \in X$ so that $x_n = y_n + z_n$, $y_n \xrightarrow{\|\cdot\|^{(0)}} 0$, and $z_n \xrightarrow{\|\cdot\|^{(1)}} 0$. Thus, $z_n = x_n - y_n \xrightarrow{\|\cdot\|^{(0)}} x$. Since $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ are consistent, $z_n \xrightarrow{\|\cdot\|^{(0)}} 0$, so $\imath\colon X_0 \to X_+$ is injective. The proof for X_1 is the same. ∎

The converse of this proposition is also true: namely, if $\|\cdot\|_+$ is a norm and the extensions of $\imath$ are injective, then $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ are consistent. The reader can familiarize himself with consistent and nonconsistent norms by doing Problem 34. The space $X_0 \cap X_1$ may be strictly larger than X, but if we replace X by this larger space and repeat the above construction, we obtain the same X_0, X_1, etc. We henceforth suppose without loss that $X = X_0 \cap X_1$.

Let S denote the closed strip $\{z \in \mathbb{C} \mid 0 \le \operatorname{Re} z \le 1\}$, S° the interior of S, and let $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ be two consistent norms on a complex vector space X. We define $\mathscr{F}(X)$ to be the set of continuous functions f from S to X_+ which are analytic in S° and which satisfy:

(i) if $\operatorname{Re} z = 0$, then $f(z) \in X_0$ and $t \to f(it)$ is continuous in $\|\cdot\|^{(0)}$; if $\operatorname{Re} z = 1$, then $f(z) \in X_1$ and $t \to f(1 + it)$ is continuous in $\|\cdot\|^{(1)}$.

(ii) $\sup_{z \in S} \|f(z)\|_+ < \infty$;

(iii) $|||f||| \equiv \sup_{t \in \mathbb{R}} \{\|f(it)\|^{(0)}, \|f(1 + it)\|^{(1)}\} < \infty$.

Proposition 4

(a) $\mathscr{F}(X)$ with the norm $|||\cdot|||$ is a Banach space.

(b) For each $t \in [0, 1]$, the subspace

$$K_t = \{f \in \mathscr{F}(X) \mid f(t) = 0\}$$

is $|||\cdot|||$-closed.

Proof $|||\cdot|||$ is clearly positive, subadditive, and positive homogeneous. By the three line theorem and the estimates $\|\cdot\|_+ \le \|\cdot\|^{(i)}$, $i = 0, 1$, we see that

$$\sup_{z \in S} \|f(z)\|_+ \le \sup_{\operatorname{Re} z = 0, 1} \|f(z)\|_+ \le |||f||| \tag{IX.20}$$

Thus $|||f||| = 0$ implies that $f \equiv 0$, so $|||\cdot|||$ is a norm on $\mathscr{F}(X)$. To see that $\mathscr{F}(X)$ is complete, let $\{f_n\}$ be a Cauchy sequence in $\mathscr{F}(X)$. By (IX.20), the functions converge uniformly to a bounded continuous function f on S. By the uniform convergence, f is analytic in S° and satisfies properties (i), (ii), and (iii). This completeness argument also shows that each of the subspaces K_t is closed. ∎

We now define

$$\tilde{X}_t = \mathscr{F}(X)/K_t, \qquad 0 \le t \le 1$$

We will denote the quotient norm on $\tilde{X}_t$ by $\|\cdot\|^{(t)}$. Notice that X may be identified with a subset of $\tilde{X}_t$ under the map which takes each $x \in X$ into $[x]$, the equivalence class of the constant function whose value is x. Further, $\tilde{X}_t$ may be identified with a subset of X_+ under the map which takes an equivalence class $[f]$ into the common value of its members at t. This map is clearly injective and the following computation shows that it is continuous: Let $[f] \in \tilde{X}_t$ and $x = f(t)$. By (IX.20), $\|x\|_+ \le |||f|||$. Thus

$$\|x\|_+ \le \inf\{|||f||| \mid f \in \mathscr{F}(X), f(t) = x\} = \|[f]\|^{(t)}$$

We now define X_t to be the completion of X in the norm $\|\cdot\|^{(t)}$. Thus, the spaces we have defined are related as follows:

$$X \to X_t \to \tilde{X}_t \to X_+$$

where each $\to$ is a continuous injective map. For $t = 0$ (respectively, $t = 1$), X_t is just the space X_0 (respectively, X_1) which we started with. To see this, let $x \in X$ and let $\|\cdot\|^{(0)}$ denote the original zero norm. If $f \in \mathscr{F}(X)$ and $f(0) = x$, then

$$\|x\|^{(0)} \leq \sup_{y \in \mathbb{R}} \{\|f(iy)\|^{(0)}, \|f(1 + iy)\|^{(1)}\} = |||f|||$$

so,

$$\|x\|^{(0)} \leq \inf\{|||f||| \mid f(0) = x\}$$

Conversely, let $c > 0$ and consider $f_c(z) = e^{-cz}x$. Then, $\|f_c(iy)\|^{(0)} = \|x\|^{(0)}$ and $\sup_{y \in \mathbb{R}} \|f_c(1 + iy)\|^{(1)}$ can be made arbitrarily small by choosing c large. Thus

$$\|x\|^{(0)} = \inf\{|||f||| \mid f(0) = x\}$$

i.e., the quotient norm is just the norm $\|\cdot\|^{(0)}$ previously defined. The proof for $t = 1$ is the same. The spaces X_t are called **interpolation spaces** between X_0 and X_1 and the norms $\|\cdot\|^{(t)}$ are called **interpolating norms** between $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$.

We remark that it is possible (though not easy, see Problem 37) to prove that $X_t = \tilde{X}_t$, but we will not need this fact. We need to know only that the norm on X_t is equal (by definition) to the quotient norm on $\mathscr{F}(X)/K_t$. Later in the examples when we will have to identify X_t with a given Banach space B_t, we will always do this by showing that both X_t and B_t are the completions of X in the same norm.

Theorem IX.20 (Calderón–Lions interpolation theorem) Let X and Y be complex vector spaces with given consistent norms $\|\cdot\|_X^{(0)}$ and $\|\cdot\|_X^{(1)}$ on X and $\|\cdot\|_Y^{(0)}$ and $\|\cdot\|_Y^{(1)}$ on Y. Suppose that $T(\cdot)$ is an analytic, uniformly bounded, continuous, $\mathscr{L}(X_+, Y_+)$-valued function on the strip S with the following properties:

(i) $T(t)\colon X \to Y$ for each $t \in (0, 1)$

(ii) For all $y \in \mathbb{R}$, $T(iy) \in \mathscr{L}(X_0, Y_0)$ and

$$M_0 = \sup_{y \in \mathbb{R}} \|T(iy)\|_{\mathscr{L}(X_0, Y_0)} < \infty$$

(iii) For all $y \in \mathbb{R}$, $T(1 + iy) \in \mathscr{L}(X_1, Y_1)$ and

$$M_1 = \sup_{y \in \mathbb{R}} \|T(1 + iy)\|_{\mathscr{L}(X_1, Y_1)} < \infty$$

Then for any $t \in (0, 1)$,

$$T(t)[X_t] \subset Y_t$$

and

$$\|T(t)\|_{\mathscr{L}(X_t, Y_t)} \leq M_0^{1-t} M_1^t$$

Proof Let $U(z) = M_0^{z-1} M_1^{-z} T(z)$. Then $U(\cdot)$ obeys the same properties as $T(\cdot)$ except that the bounds on $U(z)$ when $\operatorname{Re} z = 0$ and $\operatorname{Re} z = 1$ are equal to one. Thus, without loss of generality we may assume that $M_0 = M_1 = 1$.

If $f \in \mathscr{F}(X)$, then $T(z)f(z)$ is a continuous, bounded Y_+-valued function on S, analytic on S°. By hypotheses (ii) and (iii),

$$\|T(iy)f(iy)\|_Y^{(0)} \leq \|f(iy)\|_X^{(0)}$$
$$\|T(1 + iy)f(1 + iy)\|_Y^{(1)} \leq \|f(1 + iy)\|_X^{(1)}$$

for each $y \in \mathbb{R}$. Thus, the map $J: \mathscr{F}(X) \to \mathscr{F}(Y)$ given by $(Jf)(z) = T(z)f(z)$ has norm less than or equal to one. Furthermore, if

$$K_t^X = \{f \in \mathscr{F}(X) \mid f(t) = 0\} \qquad \text{and} \qquad K_t^Y = \{f \in \mathscr{F}(Y) \mid f(t) = 0\},$$

then $J[K_t^X] \subset K_t^Y$. Thus, J lifts to a contraction $\tilde{J}_t: \tilde{X}_t \to \tilde{Y}_t$. Since $\tilde{J}_t$ acts on equivalence classes by $\tilde{J}_t[f] = [T(t)f(t)]$, we see that $\tilde{J}_t$ equals $T(t) \restriction \tilde{X}_t$ under the natural identification of $\tilde{X}_t$ with a subset of X_+. Finally, since $T(t): X \to Y$, $T(t)[X_t] \subset Y_t$. ∎

We now present several examples which show how to apply this abstract interpolation theorem.

Example 1 (L^p spaces) Let $\langle M, \mu \rangle$ be a σ-finite measure space and suppose $1 \leq p_0 < p_1 \leq \infty$. Let $X = L^{p_0}(M, d\mu) \cap L^{p_1}(M, d\mu)$ and let $\|\cdot\|^{(0)} = \|\cdot\|_{p_0}$, $\|\cdot\|^{(1)} = \|\cdot\|_{p_1}$. We will show that $X_t = L^{p_t}(M, d\mu)$, $0 \leq t \leq 1$, where $p_t^{-1} = tp_1^{-1} + (1 - t)p_0^{-1}$, except when $p_1 = \infty$ in which case at $t = 1$, X_1 is the closure of X in the $\|\cdot\|_\infty$-norm (which may be smaller than $L^\infty(M, d\mu)$). The proof consists in showing that the $\|\cdot\|^{(t)}$-norm and the $\|\cdot\|_{p_t}$-norm agree on the simple functions which are dense in X. Let $t \in (0, 1)$ and let $\varphi(x)$ be a simple function with $\|\varphi\|_{p_t} = 1$ and define

$$f(z) = |\varphi(\cdot)|^{p_t(zp_1^{-1} + (1-z)p_0^{-1})} \exp(i \arg \varphi(\cdot))$$

Then for each $z \in S$, $f(z) \in X$, and

$$\|f(iy)\|_{L^{p_0}(M,\,d\mu)}^{p_0} = \int_M \left| |\varphi(x)|^{p_1 p_0 (iyp_1^{-1} + (1-iy)p_0^{-1})} \right| d\mu(x)$$

$$= \int_M |\varphi(x)|^{p_1}\, d\mu(x) = 1$$

If $p_1 = \infty$, $\|f(1+iy)\|_\infty = 1$ and if $p_1 < \infty$, then

$$\|f(1+iy)\|_{L^{p_1}(M,\,d\mu)}^{p_1} = \int_M \left| |\varphi(x)|^{p_1 p_1 ((1+iy)p_1^{-1} - iyp_0^{-1})} \right| d\mu(x)$$

$$= \int_M |\varphi(x)|^{p_1}\, d\mu(x) = 1$$

Therefore, $|||f||| = 1$, so $\|f(t)\|^{(t)} = \|f\|_{\mathscr{F}(X)/K_t} \leq 1$. Since the value of f at t is φ, we have $\|\varphi\|^{(t)} \leq 1$. Thus, we have shown that $\|\varphi\|^{(t)} \leq \|\varphi\|_{L^{p_t}}$ for all simple functions φ.

To prove the converse inequality, let $f \in \mathscr{F}(X)$ and let φ be a simple function on M. Let

$$g(z) = |\varphi(\cdot)|^{q_t (zq_1^{-1} + (1-z)q_0^{-1})} \exp(i \arg \varphi(\cdot))$$

where $q_t^{-1} = 1 - p_t^{-1}$. Then, since $f(z)$ is analytic and bounded as an X_+-valued function, $H(z) = \int_M f(z)g(z)\, d\mu$ is analytic and bounded in S and $H(t) = \int \varphi f(t)\, d\mu$. By the three line theorem,

$$\begin{aligned}
|H(t)| &\leq \sup_{y \in \mathbb{R}} \{|H(iy)|, |H(1+iy)|\} \\
&\leq \sup\{\|f(iy)g(iy)\|_{L^1}, \|f(1+iy)g(1+iy)\|_{L^1}\} \\
&\leq \sup_{y \in \mathbb{R}} \{\|f(iy)\|_{L^{p_0}} \|g(iy)\|_{L^{q_0}}, \|f(1+iy)\|_{L^{p_1}} \|g(1+iy)\|_{L^{q_1}}\} \\
&\leq (\sup\{\|f(iy)\|_{L^{p_0}}, \|f(1+iy)\|_{L^{p_1}}\})(\sup\{\|g(iy)\|_{L^{q_0}}, \|g(1+iy)\|_{L^{q_1}}\}) \\
&= |||f|||\cdot|||g||| \\
&= \|\phi\|_{q_t} |||f|||
\end{aligned}$$

by the above computation. Note that the above triple norms are different: one is obtained from L^{p_0} and L^{p_1}, the second from L^{q_0} to L^{q_1}. Since

$$\left| \int \varphi f(t)\, d\mu \right| \leq \|\varphi\|_{q_t} |||f|||$$

we conclude that $f \in L^{p_t}$ and

$$\|f(t)\|_{L^{p_t}} \leq |||f|||$$

It follows that for ψ simple and $f \in \psi + K_t$:

$$\|\psi\|^{(t)} = \inf_{f \in \psi + K_t} |||f|||$$

$$\geq \|\psi\|_{L^{p_t}}$$

Thus the norms $\|\cdot\|_{p_t}$ and $\|\cdot\|^{(t)}$ agree on simple functions. Since $X = L^{p_0} \cap L^{p_1}$ and the simple functions are dense in X_t and L^{p_t}, we conclude that $X_t = L^{p_t}$.

Combining the fact we have proven, namely $L^{p_t} = X_t$, with the abstract interpolation theorem we obtain:

Theorem IX.21 (the Stein interpolation theorem) Let $\langle M, \mu \rangle$ and $\langle N, \nu \rangle$ be σ-finite measure spaces and $1 \leq p_0, p_1, q_0, q_1 \leq \infty$. Suppose that $T(\cdot)$ is a continuous $\mathscr{L}(L^{p_0}(M, d\mu) + L^{p_1}(M, d\mu), L^{q_0}(N, d\nu) + L^{q_1}(N, d\nu))$-valued function on the strip $S = \{z \mid 0 \leq \operatorname{Re} z \leq 1\}$ which is uniformly bounded, analytic in the interior, and which satisfies

(i) $T(z)$: $L^{p_0} \cap L^{p_1} \to L^{q_0} \cap L^{q_1}$ for all $z \in S$.

(ii) For all $y \in \mathbb{R}$, $T(iy) \in \mathscr{L}(L^{p_0}(M, d\mu), L^{q_0}(N, d\nu))$ and

$$M_0 = \sup_{y \in \mathbb{R}} \|T(iy)\|_{\mathscr{L}(L^{p_0}, L^{q_0})} < \infty$$

(iii) For all $y \in \mathbb{R}$, $T(1 + iy) \in \mathscr{L}(L^{p_1}(M, d\mu), L^{q_1}(N, d\nu))$ and

$$M_1 = \sup_{y \in \mathbb{R}} \|T(1 + iy)\|_{\mathscr{L}(L^{p_1}, L^{q_1})} < \infty$$

Then for each $t \in (0, 1)$

$$T(t): L^{p_t}(M, d\mu) \to L^{q_t}(N, d\nu)$$

and

$$\|T(t)\|_{\mathscr{L}(L^{p_t}, L^{q_t})} \leq M_0^{1-t} M_1^t$$

where $p_t^{-1} = tp_1^{-1} + (1 - t)p_0^{-1}$, $q_t^{-1} = tq_1^{-1} + (1 - t)q_0^{-1}$.

Using the fact that $\tilde{X}_t = X$ it is possible to remove condition (i) from both the Stein and Calderón–Lions theorems. We also remark that the conclusion of the theorem still holds if only the weaker analyticity assumption, that $\int_N (T(z)\varphi)(y)\psi(y)\, d\nu(y)$ is analytic for all simple functions φ and ψ, is assumed to hold. The Riesz–Thorin theorem is an immediate corollary of the Stein interpolation theorem for we just take $T(z) = T$ for all z.

Example 2 ($\mathscr{I}_p$) Let $\mathscr{H}$ be a separable Hilbert space. Recall that the trace class $\mathscr{I}_1$ is the set of $A \in \mathscr{L}(\mathscr{H})$ so that $\mathrm{tr}(|A|) < \infty$ and that $\mathscr{I}_1$ is the dual of the compact operators $\mathrm{Com}(\mathscr{H})$ (Theorem VI.26). For $1 \leq p < \infty$, we define

$$\mathscr{I}_p = \{A \in \mathscr{L}(\mathscr{H}) \,|\, |A|^p \in \mathscr{I}_1\}$$

and set $\|A\|_p = (\mathrm{tr}(|A|^p))^{1/p}$. For $p = \infty$, we set $\mathscr{I}_\infty = \mathrm{Com}(\mathscr{H})$ with $\|A\|_\infty = \|A\|$. If $|A|^p \in \mathscr{I}_1$, then by the Riesz–Schauder theorem (Theorem VI.15) $\sigma(|A|^p)\backslash\{0\}$ consists of isolated eigenvalues of finite multiplicity. It follows that $|A|$ is compact so $A = U|A|$ is compact since $\mathrm{Com}(\mathscr{H})$ is an ideal of $\mathscr{L}(\mathscr{H})$. By Theorem VI.17, A may be represented as $A = \sum_{n=1}^{N} \lambda_n(\psi_n, \cdot)\varphi_n$ where $\{\psi_n\}$ and $\{\varphi_n\}$ are orthonormal sets and the λ_n are the singular values of A (nonzero eigenvalues of $|A|$). Thus,

$$|A| = \sum_{n=1}^{N} \lambda_n(\psi_n, \cdot)\psi_n \qquad \text{and} \qquad |A|^p = \sum_{n=1}^{N} \lambda_n^p(\psi_n, \cdot)\psi_n$$

so

$$\|A\|_p = (\mathrm{tr}(|A|^p))^{1/p} = \left(\sum_{n=1}^{N} \lambda_n^p\right)^{1/p}$$

That is, $\mathscr{I}_p$ is just the set of compact operators whose singular values are in ℓ_p and the norms are equal. This remains true even if $p = \infty$.

Proposition 5 Let $1 \leq p \leq \infty$ and $q^{-1} + p^{-1} = 1$. If $A \in \mathscr{I}_p$ and $B \in \mathscr{I}_q$, then $AB \in \mathscr{I}_1$ and $\|AB\|_1 \leq \|A\|_p \|B\|_q$.

Proof For $p = 1$, $q = \infty$, this is just Problem 28 of Chapter VI. For $1 < p < \infty$, the proof is similar to the proof of the Hölder inequality given in Proposition 2: Let $A = U|A|$ and $B = V|B|$ be the polar decompositions of A and B and define

$$F(z) = \mathrm{tr}(U|A|^{pz}V|B|^{q(1-z)})$$

$F(z)$ is bounded and continuous on the strip $S = \{z \,|\, 0 \leq \mathrm{Re}\, z \leq 1\}$ and analytic in the interior. Since $|A|^{pz}$ is unitary on the line $\mathrm{Re}\, z = 0$ and $|B|^{q(1-z)}$ is unitary on the line $\mathrm{Re}\, z = 1$,

$$\begin{aligned} |F(iy)| &= |\mathrm{tr}(U|A|^{iyp}V|B|^q|B|^{iyq})| \\ &\leq \mathrm{tr}(|B|^q) = \|B\|_q^q \\ |F(1+iy)| &= |\mathrm{tr}(U|A|^p|A|^{iyp}V|B|^{-iyq})| \\ &\leq \mathrm{tr}(|A|^p) = \|A\|_p^p \end{aligned}$$

We have used the properties of the trace that $\operatorname{tr}(CD) = \operatorname{tr}(DC)$ and $|\operatorname{tr}(CD)| \leq \|D\| \operatorname{tr}(C)$ if $C \geq 0$. Thus, by the three line theorem $|F(z)| \leq \|A\|_p^{pz} \|B\|_q^{q(1-z)}$ for all z in $(0, 1)$. In particular, for $z = p^{-1}$, we find

$$|\operatorname{tr}(AB)| = \left|F\left(\frac{1}{p}\right)\right| \leq \|A\|_p \|B\|_q \quad \blacksquare$$

Suppose that $A = U|A| \in \mathscr{I}_p$ and define $B = |A|^{p-1}U^* \|A\|_p^{-p/q}$. Then

$$\begin{aligned}
\|B\|_q &= \operatorname{tr}[\,|\,|A|^{p-1}U^*|^q]^{1/q} \|A\|_p^{-p/q} \\
&= \operatorname{tr}[(U|A|^{2(p-1)}U^*)^{q/2}]^{1/q} \|A\|_p^{-p/q} \\
&= \operatorname{tr}[U|A|^{q(p-1)}U^*]^{1/q} \|A\|_p^{-p/q} \\
&= \operatorname{tr}[\,|A|^{q(p-1)}]^{1/q} \|A\|_p^{-p/q} \\
&= 1
\end{aligned}$$

since $\operatorname{Ker} U = \operatorname{Ker} A$. A similar computation shows that $\operatorname{tr}(AB) = \|A\|_p$. Thus, by Proposition 5,

$$\|A\|_p = \sup_{\|D\|_q = 1} |\operatorname{tr}(AD)|$$

Now, suppose that A and C are in $\mathscr{I}_p$. Then

$$\begin{aligned}
\|A + C\|_p &= \sup_{\|D\|_q = 1} |\operatorname{tr}((A + C)D)| \\
&\leq \sup_{\|D\|_q = 1} |\operatorname{tr}(AD)| + \sup_{\|D\|_q = 1} |\operatorname{tr}(CD)| \\
&= \|A\|_p + \|C\|_p
\end{aligned}$$

Thus $\mathscr{I}_p$ is a vector space and $\|\cdot\|_p$ is a norm on $\mathscr{I}_p$.

Proposition 6 Let $1 \leq p \leq \infty$. Then

(a) $\mathscr{I}_p$ is a Banach space with norm $\|\cdot\|_p$.
(b) $\mathscr{I}_1 \subset \mathscr{I}_p \subset \operatorname{Com}(\mathscr{H})$ and $\mathscr{I}_p$ is the closure of the finite rank operators in the norm $\|\cdot\|_p$.
(c) If $A \in \mathscr{I}_p$, then $A^* \in \mathscr{I}_p$ and $\|A^*\|_p = \|A\|_p$.

Proof For $p = \infty$, (a), (b), and (c) are standard properties of the compact operators. So, suppose $1 \leq p < \infty$. For any sequence $\{\lambda_n\}$,

$$\|\{\lambda_n\}\|_\infty \leq \|\{\lambda_n\}\|_p \leq \|\{\lambda_n\}\|_1$$

so

$$\|A\| \leq \|A\|_p \leq \|A\|_1$$

Thus any Cauchy sequence $\{A_n\}$ in $\mathscr{I}_p$ converges in the uniform norm to a limiting operator A. The reader can easily check for himself that $A \in \mathscr{I}_p$

and $\|A_n - A\|_p \to 0$. Therefore, $\mathscr{I}_p$ is complete in the norm $\|\cdot\|_p$. As indicated above, each $A \in \mathscr{I}_p$ is compact and $\|A\|_p = \|\{\lambda_n\}\|_{\ell_p}$ where the $\{\lambda_n\}$ are the singular values of A in the representation $A = \sum_{n=1}^{\infty} \lambda_n(\psi_n, \cdot)\varphi_n$. Thus, the finite rank operators $A_M = \sum_{n=1}^{M} \lambda_n(\psi_n, \cdot)\varphi_n$ converge to A in the $\|\cdot\|_p$-norm. The inclusions $\mathscr{I}_1 \subset \mathscr{I}_p \subset \mathrm{Com}(\mathscr{H})$ follow immediately from the above inequality. This proves (a) and (b).

To prove (c) we observe that A and A^* have the same singular values. ∎

Proposition 7 If $1 < p, q < \infty$ and $p^{-1} + q^{-1} = 1$, then $\mathscr{I}_p^* = \mathscr{I}_q$.

Proof Proposition 5 and the remark thereafter show that for each $A \in \mathscr{I}_q$ the map $B \to \mathrm{tr}(AB)$ is a bounded linear functional on $\mathscr{I}_p$ of norm $\|A\|_q$. Conversely, let $\Lambda \in \mathscr{I}_p^*$. Then since $\|A\|_p \leq \|A\|_1$, $\Lambda \in \mathscr{I}_1^*$ so by Theorem VI.26 there is an $A \in \mathscr{L}(\mathscr{H})$ so that $\Lambda(B) = \mathrm{tr}(AB)$ for all $B \in \mathscr{I}_1$. We want to show that $A \in \mathscr{I}_q$. A may be written $D + iC$ where D and C are self-adjoint. Since

$$|\mathrm{tr}(A^*B)| = |\mathrm{tr}(AB^*)| \leq \|\Lambda\| \, \|B^*\|_p = \|\Lambda\| \, \|B\|_p$$

we have

$$|\mathrm{tr}(DB)| \leq \|\Lambda\| \, \|B\|_p, \qquad |\mathrm{tr}(CB)| \leq \|\Lambda\| \, \|B\|_p$$

Thus it is sufficient to prove that $A \in \mathscr{I}_q$ in the case where A is self-adjoint. Let $a > 0$ and $E(a, \infty)$ be the spectral projections of A corresponding to the interval (a, ∞). Suppose $E(a, \infty)$ is infinite dimensional and let $\{\varphi_n\}$ be an orthonormal basis for $E(a, \infty)$. If we define

$$B_M = \left(\sum_{n=1}^{M} \frac{1}{n} P_{\varphi_n}\right)\left(\sum_{n=1}^{M} \frac{1}{n^p}\right)^{-1/p}$$

where P_{φ_n} is the projection onto φ_n, we have $\|B_M\|_p = 1$. But

$$\mathrm{tr}(AB_M) \geq \left(\sum_{n=1}^{M} \frac{a}{n}\right)\left(\sum_{n=1}^{M} \frac{1}{n^p}\right)^{-1/p} \xrightarrow{M \to \infty} \infty$$

which contradicts the fact that $|\mathrm{tr}(AB_M)| \leq \|\Lambda\|$. Thus, $E(a, \infty)$ is finite dimensional and a similar proof shows that $E(-\infty, -a)$ is finite dimensional. It follows that A is compact and therefore may be represented as $A = \sum_{n=1}^{\infty} \mu_n P_{\psi_n}$ for some orthonormal set $\{\psi_n\}$. If $\{\gamma_n\}_{n=1}^{M}$ is any finite sequence so that $(\sum_1^M |\gamma_n|^p)^{1/p} = 1$, then $B_\gamma = \sum_1^M \gamma_n P_{\psi_n} \in \mathscr{I}_p$ and

$$\left|\sum_1^M \gamma_n \mu_n\right| = |\mathrm{tr}(AB_\gamma)| \leq \|\Lambda\|$$

so $\{\mu_n\} \in \ell_q$ since $\ell_q = \ell_p^*$. Thus, $(\mathrm{tr}(|A|^q))^{1/q} = (\sum |\mu_n|^q)^{1/q} < \infty$ and $A \in \mathscr{I}_q$. ∎

Proposition 8 Let $1 \le p_0 < p_1 \le \infty$ and define $X = \mathscr{I}_{p_0}$. Then $\|\cdot\|^{(0)} = \|\cdot\|_{p_0}$ and $\|\cdot\|^{(1)} = \|\cdot\|_{p_1}$ are consistent norms on X and $X_t = \mathscr{I}_{p_t}$ where $p_t = tp_1^{-1} + (1-t)p_0^{-1}$.

We omit the proof of Proposition 8; it is almost identical to the proof in Example 1 except that the decomposition $\varphi(x) = |\varphi(x)| \exp(i \arg \varphi(x))$ is replaced by the decomposition $A = U|A|$ and the integral is replaced by the trace.

Theorem IX.22 Let $\mathscr{H}_1$ and $\mathscr{H}_2$ be separable Hilbert spaces with corresponding spaces $\mathscr{I}_p^{(1)}$, $\mathscr{I}_q^{(2)}$ of operators. Suppose that T takes $\mathscr{F}_1$, the finite rank operators on $\mathscr{H}_1$, into $\mathrm{Com}(\mathscr{H}_2)$, and that

(i) $\|T(A)\|_{q_0} \le M_0 \|A\|_{p_0}$ for all $A \in \mathscr{F}_1$.
(ii) $\|T(A)\|_{q_1} \le M_1 \|A\|_{p_1}$ for all $A \in \mathscr{F}_1$.

Then $\|T(A)\|_{q_t} \le M_1^t M_0^{1-t} \|A\|_{p_t}$ for all $A \in \mathscr{F}_1$ so T extends uniquely to a bounded map of $\mathscr{I}_{p_t}$ into $\mathscr{I}_{q_t}$ where $p_t^{-1} = tp_1^{-1} + (1-t)p_0^{-1}$ and $q_t^{-1} = tq_1^{-1} + (1-t)q_0^{-1}$.

Proof The theorem follows immediately from Proposition 8 and the Calderón–Lions interpolation theorem. ∎

Example 3 (rigged Hilbert spaces) Let $\mathscr{H}$ be a Hilbert space and suppose that A is a positive self-adjoint operator on $\mathscr{H}$ with $\mathrm{Ker}\, A = \{0\}$ so that A^{-1} is also self-adjoint (both A and A^{-1} may be unbounded). Let $X = C^\infty(A) \cap C^\infty(A^{-1})$ and for each $m \in \mathbb{R}$, let $\mathscr{H}_m$ be the completion of X in the norm $\|\varphi\|_m = \|A^{m/2}\varphi\|_{\mathscr{H}}$. By the spectral theorem we may assume that $\mathscr{H} = L^2(M, d\mu)$ where $\langle M, \mu\rangle$ is a measure space and A is multiplication by a function $f \ge 0$. Clearly, $\mathscr{H}_m = L^2(M, f^m\, d\mu)$, and a short argument shows that the norms $\|\cdot\|_m$ are consistent. Let m_0 and m_1 be fixed, $m_t = tm_1 + (1-t)m_0$. Then a similar proof to that in Example 1 shows that $X_t = \mathscr{H}_{m_t}$. The proof that $\mathscr{H}_{m_t} \subset X_t$ uses the function $F(z) = f(\cdot)^{zm_1 + (1-z)m_0}$. The proof that $X_t \subset \mathscr{H}_{m_t}$ uses the natural identification of $\mathscr{H}_m^*$ with $\mathscr{H}_{-m}$. The reader is asked to provide the details in Problem 35. Once one has identified X_t as H_{m_t}, the abstract interpolation theorem can be applied to make concrete statements about operators on $\mathscr{H}$. Here are two simple examples:

Proposition 9 Let A and B be positive self-adjoint operators with (possibly unbounded) inverses on a Hilbert space $\mathscr{H}$. Let T be a bounded linear transformation of $\mathscr{H}$ into itself which satisfies:

(i) $\|T\varphi\| \leq M_0\|\varphi\|$ for all $\varphi \in \mathscr{H}$.
(ii) $T: D(A^2) \to D(B^2)$ and $\|B^2T\varphi\| \leq M_1\|A^2\varphi\|$ for all $\varphi \in D(A^2)$.

Then $T: D(A) \to D(B)$ and

$$\|BT\varphi\| \leq M_0^{1/2}M_1^{1/2}\|A\varphi\| \qquad \text{for all } \varphi \in D(A)$$

Proposition 10 For $m \in \mathbb{R}$ let W_m be the mth Sobolev space (defined in Section IX.6). Suppose that $g \in C^k$ and $D^\alpha g$ is bounded for all α with $|\alpha| \leq k$. Then, for each m with $|m| \leq k$, $f \mapsto gf$ is a bounded map of W_m into W_m.

Proof We first show that $g: W_k \to W_k$ is bounded. By Proposition 1 of Section IX.6, $f \in W_k$ if and only if $D^\alpha f \in L^2$ for all $|\alpha| \leq k$. From this it follows easily that the norm $\|f\|_{k,2} = \sum_{|\alpha| \leq k} \|D^\alpha f\|_{L^2}$ is equivalent to the norm $\|f\|_k$ on W_k. By Leibnitz's rule and the fact that the derivatives of g are bounded we have

$$\|gf\|_{k,2} = \sum_{|\alpha| \leq k} \|D^\alpha gf\|_2 \leq C \sum_{|\alpha| \leq k} \|D^\alpha f\|_2 = C\|f\|_{k,2}$$

Thus $g: W_k \to W_k$ is bounded. By duality, $g: W_{-k} \to W_{-k}$ is bounded. The spaces W_m are the rigged Hilbert spaces associated with the operator $-\Delta + I$, so by the interpolation theorem, $g: W_m \to W_m$ is bounded for each m with $|m| \leq k$. ∎

For another application of the $\mathscr{H}_m$-interpolation theorem, see the proof of Theorem X.18. For another illustration of interpolating spaces, see Problem 36.

IX.5 Fundamental solutions of partial differential equations with constant coefficients

In this section and the next we will describe two applications of the Fourier transform to the study of partial differential equations. This is not a book about partial differential equations though we have touched on the subject from time to time, so our purpose here is neither to discuss in detail the techniques nor give the strongest results, but to illustrate and explain the application of the methods of functional analysis.

As in Chapter V, $p(x)$ denotes a polynomial in several variables $x = \langle x_1, \ldots, x_n \rangle$, and $p(D)$ denotes the partial differential operator obtained by substituting $\partial/\partial x_i$ for x_i wherever it occurs in $p(x)$.

Definition A **fundamental solution** for the partial differential operator $p(D)$ is a distribution $E \in \mathscr{D}'$ so that $p(D)E = \delta$.

The reason for studying fundamental solutions is that if we define $u = E * f$ where $f \in C_0^\infty(\mathbb{R}^n)$, then

$$\begin{aligned} p(D)u = p(D)(E * f) &= p(D)E * f \\ &= \delta * f \\ &= f \end{aligned}$$

Thus, if we can find a fundamental solution, then we have an existence theorem for all the partial differential equations $p(D)u = f$ where $f \in C_0^\infty(\mathbb{R}^n)$. Furthermore, if we can find an expression for E, then we have an explicit representation of a solution, namely $u = E * f$.

Example (Poisson's equation) For Poisson's equation, $\Delta u = f$, in three dimensions, the function $E(\mathbf{r}) = -1/4\pi r$ is a fundamental solution. This can be seen as follows: We denote by B_ε the ball about zero of radius ε. Let $\varphi \in C_0^\infty(\mathbb{R}^3)$. Then

$$\begin{aligned} (\Delta E)(\varphi) = E(\Delta\varphi) &= -\int_{\mathbb{R}^3} \frac{1}{4\pi r} \Delta\varphi \, dx \\ &= \lim_{\varepsilon \downarrow 0} -\int_{\mathbb{R}^3 \setminus B_\varepsilon} \frac{1}{4\pi r} \Delta\varphi \, dx \\ &= \lim_{\varepsilon \downarrow 0} \left\{ \int_{\mathbb{R}^3 \setminus B_\varepsilon} -\Delta\left(\frac{1}{4\pi r}\right)\varphi \, dx + \int_{\partial B_\varepsilon} \frac{1}{4\pi r} \frac{\partial}{\partial r} \varphi \, dS - \int_{\partial B_\varepsilon} \varphi \frac{\partial}{\partial r}\left(\frac{1}{4\pi r}\right) dS \right\} \end{aligned}$$

where dS denotes the usual measure on the surface ∂B_ε of B_ε. The first term on the right-hand side equals zero. The second term converges to zero and the third term converges to $\varphi(0)$ as $\varepsilon \downarrow 0$ because φ is continuous at zero. Thus $\Delta E(\varphi) = \varphi(0)$ so $\Delta E = \delta$.

In order to see the difficulties in finding fundamental solutions, let us work formally for a moment. We would like to solve the partial differential equation $p(D)E = \delta$. Taking the Fourier transform of both sides we obtain $p(ix)\hat{E} = (2\pi)^{-n/2}$, so we expect

$$E = \widehat{((2\pi)^{n/2} p(ix))^{-1}}$$

If $p(ix)$ has no real zeros, then we can use the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$ to define E. However, $p(ix)$ is a polynomial in several variables and may have whole manifolds of zeros. Thus $p(ix)^{-1}$ may not be locally integrable in which case $\int p(ix)^{-1}\varphi(x)\,dx$ does not make sense as it stands,

so we cannot immediately interpret $p(ix)^{-1}$ as a distribution. This is reminiscent of the situation in Examples 6 and 9 of Section V.3 where the function $1/x$ in one variable could not be immediately interpreted as a distribution since it is not locally integrable. Even in that simple case, a limiting procedure was required. As in that case, we expect that different limiting procedures will give different distributions. In fact, in general, partial differential equations will have many fundamental solutions in $\mathscr{D}'$, and sometimes have more than one in $\mathscr{S}'(\mathbb{R}^n)$.

The Malgrange–Ehrenpreis theorem states that every constant coefficient partial differential operator $p(D)$ has a fundamental solution. The proof depends on a complex-variables argument and the Hahn–Banach theorem. Before giving a sketch of the proof, we will illustrate the Hahn–Banach part of the argument by a simple example. Consider the operator $I - \Delta$. In this case $p(ix) = 1 + x^2$ has no zeros, so $\hat{E} = \{(2\pi)^{n/2}(1 + x^2)\}^{-1}$ is a well-defined tempered distribution and E satisfies $(I - \Delta)E = \delta$. We now give another argument which proves the existence of E without using the fact that we have extended the Fourier transform to $\mathscr{S}'$. Let $\varphi \in C_0^\infty(\mathbb{R}^n)$. Then

$$\begin{aligned} |\delta_0(\varphi)| = |\varphi(0)| &\le \|\varphi\|_\infty \\ &\le \|\hat{\varphi}\|_1 \\ &= \|(1 + |\lambda|^2)^m \hat{\varphi}(\lambda)(1 + |\lambda|^2)^{-m}\|_1 \\ &\le C\|(1 + |\lambda|^2)^m \hat{\varphi}(\lambda)\|_2 \end{aligned}$$

where we have chosen m large enough so that $(1 + |\lambda|^2)^{-m} \in L^2(\mathbb{R}^n)$. Using (IX.1) and the Plancherel theorem, we have

$$\|(1 + |\lambda|^2)^m \hat{\varphi}(\lambda)\|_2 = \|(1 - \Delta)^m \varphi\|_2$$

and thus

$$|\varphi(0)| \le C\|(1 - \Delta)^m \varphi\|_2 \tag{IX.21}$$

Therefore, the map $\tilde{T}$ from $(I - \Delta)^m[C_0^\infty(\mathbb{R}^n)]$ to $\mathbb{C}$ given by

$$\tilde{T}: (1 - \Delta)^m \varphi \to \varphi(0)$$

is well defined and bounded in the L^2-norm. By the Hahn–Banach theorem $\tilde{T}$ can be extended from $(I - \Delta)^m C_0^\infty(\mathbb{R}^n)$ to a bounded linear functional T on all of $L^2(\mathbb{R}^n)$. It follows from the Riesz lemma that there is a $t(x) \in L^2(\mathbb{R}^n)$ so that

$$\begin{aligned} \delta(\varphi) = \varphi(0) = T((I - \Delta)^m \varphi) \\ = \int t(x)(1 - \Delta)^m \varphi \, dx \\ = [(1 - \Delta)^{m-1} T]((1 - \Delta)\varphi) \end{aligned}$$

If we set $E = (1 - \Delta)^{m-1}T$, then clearly $(1 - \Delta)E = \delta$.

We are ready to state the Malgrange–Ehrenpreis theorem and sketch the proof.

Theorem IX.23 For every constant coefficient partial differential operator, $p(D)$, on $\mathbb{R}^n$, there is a distribution $E \in \mathscr{D}'$ so that $p(D)E = \delta$.

Proof Define $p^*(x) = p(-x)$ and $q(x) = p^*(ix)$ and let $\varphi \in C_0^\infty(\mathbb{R}^n)$. From the Paley-Wiener theorem we know that for each $y \in \mathbb{R}^n$,

$$\widehat{(p^*(D)\varphi)}(y + \zeta) = \hat{\varphi}(y + \zeta)q(y + \zeta)$$

is an entire function of $\zeta \in \mathbb{C}^n$. Let $Q(x) = \sum_\alpha |D^\alpha q(x)|$; notice that Q is positive and bounded away from zero. The first step in the proof uses the Cauchy integral formula to show that

$$|Q(x)\hat{\varphi}(x)| \leq C_1 \int_{|\zeta| \leq \varepsilon} |\hat{\varphi}(x + \zeta)q(x + \zeta)|\, d^{2n}\zeta$$

$$= C_1 \int_{|\zeta| \leq \varepsilon} |\widehat{p^*(D)\varphi}(x + \zeta)|\, d^{2n}\zeta$$

where C_1 depends on ε but is independent of φ and $d^{2n}\zeta$ is Lebesgue measure on $\mathbb{C}^n$. This complex-variable argument is outlined in Problem 41.

Using the above estimate, we have

$$|\varphi(0)| \leq (2\pi)^{-n/2} \int_{\mathbb{R}^n} |\hat{\varphi}(y)|\, dy$$

$$\leq C_2 \int_{\mathbb{R}^n} \left(\int_{|\zeta| \leq \varepsilon} |\widehat{p^*(D)\varphi}(y + \zeta)|\, |Q(y)|^{-1}\, d^{2n}\zeta \right) dy$$

$$= C_2 \int_{\mathbb{R}^n} \int_{|\lambda|^2 + |\mu|^2 \leq \varepsilon^2} |\widehat{p^*(D)\varphi}(y + \lambda + i\mu)|\, |Q(y)|^{-1}\, d\lambda\, d\mu\, dy$$

For $|\lambda| \leq \varepsilon$, $Q(y + \lambda)(Q(y))^{-1} \leq C_3$ independently of y, so

$$|\varphi(0)| \leq C_4 \int_{\mathbb{R}^n} \int_{|\lambda|^2 + |\mu|^2 \leq \varepsilon^2} |\widehat{p^*(D)\varphi}(y + \lambda + i\mu)|\, (Q(y + \lambda))^{-1}\, d\lambda\, d\mu\, dy$$

$$\leq C_5 \int_{\mathbb{R}^n} \int_{|\mu|^2 \leq \varepsilon^2} |\widehat{p^*(D)\varphi}(y + i\mu)|\, (Q(y))^{-1}\, d\mu\, dy \qquad \text{(IX.22)}$$

This estimate takes the place of the simple a priori estimate (IX.21) in the above example (all the C_i depend on ε but are independent of φ).

From here on the structure of the argument is the same as in the example. Let

$$\|\varphi\|_Q = \int_{\mathbb{R}^n} \int_{|\mu|^2 \le \varepsilon^2} |\hat{\varphi}(y + i\mu)(Q(y))^{-1}| \, d\mu \, dy$$

We first show that $\|\cdot\|_Q$ is a continuous norm on $\mathscr{D}$. Since Q is bounded from below

$$\begin{aligned} \|\varphi\|_Q &\le C_6 \int_{\mathbb{R}^n} \int_{|\mu| \le \varepsilon} |\hat{\varphi}(y + i\mu)| \, d\mu \, dy \\ &\le C_7 \sup_{\substack{y \in \mathbb{R}^n \\ |\mu| \le \varepsilon}} |(1 + y^2)^{n+1} \hat{\varphi}(y + i\mu)| \\ &\le C_7 \sup_{|\mu| \le \varepsilon} \|(I - \Delta)^{n+1} e^{\mu \cdot x} \varphi(x)\|_1 \end{aligned}$$

The right-hand side is a continuous norm on $C_0^\infty(K)$ for each compact set $K \subset \mathbb{R}^n$. Since $\mathscr{D}$ has the inductive limit topology, $\|\cdot\|_Q$ is a continuous norm on $\mathscr{D}$. The basic estimate (IX.22) shows that the map

$$\tilde{E}\colon p^*(D)\varphi \to \varphi(0)$$

is well-defined. That is, if $p^*(D)\varphi_1 = p^*(D)\varphi_2$, then $\varphi_1(0) = \varphi_2(0)$. $\tilde{E}$ is continuous since $\|\cdot\|_Q$ is a continuous norm. Thus by the Hahn–Banach theorem there is an E in $\mathscr{D}'$ which extends $\tilde{E}$. Since

$$(p(D)E)(\varphi) = E(p^*(D)\varphi) = \varphi(0)$$

we have found a fundamental solution for $p(D)$. ∎

IX.6 Elliptic regularity

I turn away with fear and horror from this lamentable plague of functions which do not have derivatives. — *Hermite, in a letter to Stieltjes*

Suppose that u is a weak solution of $-\Delta u = g$ in a region Ω. Our main goal in this section is to prove that if g is C^∞ in Ω, then u is C^∞ in Ω also. This theorem, known as Weyl's lemma, has many important generalizations. We restrict ourselves here to a proof of Weyl's lemma, leaving a discussion of the generalizations to the notes. The importance of these so-called "regularity" theorems is that they provide the second step in the proof

that certain classes of elliptic partial differential equations have strict solutions. One first uses the Hahn–Banach theorem or a self-adjointness argument to prove the existence of a weak solution (see Section IX.5 or X.3), and then uses a regularity theorem to prove that any weak solution is a strict solution. In Section V.4 we noted that $u_{tt} - u_{xx} = 0$ has many weak solutions which are *not* strict solutions. The difference between the two cases $u_{tt} - u_{xx} = 0$ and $u_{tt} + u_{xx} = 0$ lies in the fact that the polynomials xt, x, t, and 1 can all be bounded by $C(x^2 + t^2)$ but not by $C(x^2 - t^2)$. The reader will see how such estimates enter into the proof. Although a regularity theorem of the C^∞-type (or even the C^k-type) does not hold for non-elliptic partial differential equations, there is a weaker regularity theorem which we discuss in the Notes to Section IX.10.

The proof of Weyl's lemma itself is divided into two parts. The first is to show that if $-\Delta u = g$ and if all the weak derivatives of g of order less than or equal to m are L^2 functions, then all the weak derivatives of u of order less than or equal to $m + 2$ are L^2 functions. The second part, known as Sobolev's lemma, shows that any function in $L^2(\mathbb{R}^n)$ which has $k > (n/2) + \sigma$ weak derivatives in $L^2(\mathbb{R}^n)$ is equal (a.e.) to a function in C^σ. Weyl's lemma results from combining these two parts with the assumption that g is C^∞.

We begin by introducing the Sobolev spaces and several of their important properties.

Definition A distribution $T \in \mathscr{S}'(\mathbb{R}^n)$ is said to be in W_m, the ***m*th Sobolev space** ($m \in \mathbb{R}$) if $\hat{T}$ is a measurable function and

$$\|T\|_m^2 = \int (1 + |\lambda|^2)^m |\hat{T}(\lambda)|^2 \, d\lambda < \infty$$

W_m is a Hilbert space under the norm $(T, T)^{1/2} = \|T\|_m$. As in the discussion of quadratic forms in Section VIII.6, it is useful to suppress the correspondence between W_m^* and W_m given by the Riesz lemma. Instead we identify W_m^* and W_{-m} by associating $T \in W_{-m}$ with the functional on W_m given by

$$T(S) = \int \hat{T}(-\lambda)\hat{S}(\lambda) \, d\lambda$$

This identification is natural since it agrees with the meaning of $T(\varphi)$ when $\varphi \in \mathscr{S}(\mathbb{R}^n)$ and T is viewed as an element of $\mathscr{S}'(\mathbb{R}^n)$.

Proposition 1 If m is a nonnegative integer, then $f \in W_m$ if and only if $D^\alpha f \in L^2(\mathbb{R}^n)$ for all α satisfying $|\alpha| \leq m$, where $D^\alpha f$ means the derivative in the sense of distributions.

Proof By Theorem IX.2, $\widehat{D^\alpha T} = (i\lambda)^\alpha \hat{T}$ for all T in $\mathscr{S}'(\mathbb{R}^n)$. If $T \in W_m$, then $(i\lambda)^\alpha \hat{T} \in L^2(\mathbb{R}^n)$ if $|\alpha| \leq m$, so by the Plancherel theorem $D^\alpha T \in L^2(\mathbb{R}^n)$. Conversely, if $D^\alpha T \in L^2(\mathbb{R}^n)$ for all α with $|\alpha| \leq m$, then $(i\lambda)^\alpha \hat{T} = \widehat{D^\alpha T} \in L^2(\mathbb{R}^n)$ if $|\alpha| \leq m$, so $T \in W_m$. ∎

Proposition 2 Let m be an integer. If $T \in W_m$ and $\varphi \in C^{|m|}$ with bounded derivatives, then $\varphi T \in W_m$.

Proof If $m \geq 0$, then the conclusion follows from Leibnitz's rule and Proposition 1. If $m < 0$, multiplication by φ on W_m is the adjoint of multiplication by φ on $W_{|m|}$ under the natural identification of W_m and $W_{|m|}^*$. Thus multiplication by φ is bounded. ∎

The above proposition is a special case of Proposition 10 in the Appendix to Section IX.4. We have repeated the proof since this part of Proposition 10 does not need interpolation.

Definition Let Ω be an open subset of $\mathbb{R}^n$. The **local Sobolev space** $W_m(\Omega)$ is the set of distributions $T \in \mathscr{D}'(\mathbb{R}^n)$ so that $\varphi T \in W_m$ for all $\varphi \in C_0^\infty(\mathbb{R}^n)$ with support in Ω.

The useful property of the local Sobolev spaces is:

Proposition 3 If Ω is an open *bounded* region in $\mathbb{R}^n$, then every $T \in \mathscr{D}'(\mathbb{R}^n)$ is in $W_m(\Omega)$ for some m. That is, $\mathscr{D}'(\mathbb{R}^n) = \bigcup_{m=-\infty}^{\infty} W_m(\Omega)$.

Proof Let η be a function in $C_0^\infty(\mathbb{R}^n)$ which is identically one on $\overline{\Omega}$. Since ηT is a distribution with compact support, $|(\widehat{\eta T})(\lambda)| \leq C(1 + |\lambda|)^M$ for some M by Theorem IX.12. Thus, if p is an integer larger than $M + (n/2)$, $\eta T \in W_{-p}$. By Proposition 2, if $\varphi \in C_0^\infty(\mathbb{R}^n)$ with supp $\varphi \subset \Omega$, then $\varphi T = \varphi \eta T \in W_{-p}$ also. Thus $T \in W_{-p}(\Omega)$. ∎

We are now prepared for the first part of the proof of Weyl's lemma.

Lemma Let $T \in \mathscr{D}'(\mathbb{R}^n)$ and Ω be an open set in $\mathbb{R}^n$.

(a) If $T \in W_m$ and $-\Delta T \in W_m$, then $T \in W_{m+2}$. Furthermore, if $T \in W_m$, then $\partial T/\partial x_j \in W_{m-1}$.
(b) If $T \in W_m(\Omega)$ and $-\Delta T \in W_m(\Omega)$, then $T \in W_{m+2}(\Omega)$.
(c) If $T \in W_m$ and m is an integer, then $T \in W_m(\Omega)$.

Proof To prove (a), notice that if $T \in W_m$, then $(1 + |\lambda|^2)^{m/2}\hat{T} \in L^2(\mathbb{R}^n)$; and if $-\Delta T \in W_m$, then $|\lambda|^2(1 + |\lambda|^2)^{m/2}\hat{T} \in L^2(\mathbb{R}^n)$. Thus

$$(1 + |\lambda|^2)^{(m/2)+1}\hat{T} \in L^2(\mathbb{R}^n),$$

so $T \in W_{m+2}$. Further, if $T \in W_m$, then $\lambda_j(1 + |\lambda|^2)^{(m-1)/2}\hat{T} \in L^2(\mathbb{R}^n)$, so $\partial T/\partial x_j \in W_{m-1}$.

To prove (b), we first note that Leibnitz's rule holds for the product of a distribution and a function, i.e.

$$\frac{\partial}{\partial x_j}(\varphi T) = \left(\frac{\partial \varphi}{\partial x_j}\right)T + \varphi \frac{\partial T}{\partial x_j} \tag{IX.23}$$

$$-\Delta(\varphi T) = (-\Delta\varphi)T - 2\sum \frac{\partial \varphi}{\partial x_j}\frac{\partial T}{\partial x_j} - \varphi\, \Delta T \tag{IX.24}$$

Now, suppose T and $-\Delta T$ are in $W_m(\Omega)$. If $\varphi \in C_0^\infty(\Omega)$, then by (IX.23) and part (a), $\varphi\, \partial T/\partial x_j \in W_{m-1}$. Thus, by (IX.24), $-\Delta(\varphi T) \in W_{m-1}$, so by part (a) we conclude that $\varphi T \in W_{m+1}$. We now use (IX.23) again obtaining $\varphi\, \partial T/\partial x_j \in W_m$ and (IX.24) again obtaining $-\Delta(\varphi T) \in W_m$. Thus, it follows from part (a) that $\varphi T \in W_{m+2}$. Since $\varphi \in C_0^\infty(\Omega)$ was arbitrary, $T \in W_{m+2}(\Omega)$. This proves (b).

(c) follows from Proposition 2. ∎

Theorem IX.24 (Sobolev's lemma) Let $T \in \mathscr{D}'(\mathbb{R}^n)$ and let Ω be an open set in $\mathbb{R}^n$. Suppose that $T \in W_m(\Omega)$, where $m > n/2$ and let ℓ be a non-negative integer satisfying $\ell < m - (n/2)$. Then on Ω, T is equal to a C^ℓ function.

Proof We begin with the case where $\Omega = \mathbb{R}^n$. Since $T \in W_m$,

$$(1 + |\lambda|^2)^{m/2}\hat{T} \in L^2(\mathbb{R}^n).$$

Thus, since $(1 + |\lambda|^2)^{-(n/4)-\varepsilon}$ is also in $L^2(\mathbb{R}^n)$ for each $\varepsilon > 0$, we conclude that

$$(1 + |\lambda|^2)^{-(n/4)-\varepsilon}(1 + |\lambda|^2)^{m/2}\hat{T}(\lambda) \in L^1(\mathbb{R}^n)$$

Therefore, whenever $|\alpha| \leq \ell$

$$|\lambda^\alpha \hat{T}(\lambda)| \leq |\lambda|^\ell(1 + |\lambda|^2)^{-(m/2)+(n/4)+\varepsilon}G(\lambda)$$

where $G \in L^1(\mathbb{R}^n)$. Since we can choose $\varepsilon > 0$ so that $\ell < m - (n/2) - 2\varepsilon$, $\lambda^\alpha \hat{T} \in L^1(\mathbb{R}^n)$ for each $|\alpha| \le \ell$. By the Riemann–Lebesgue lemma,

$$T(x) = (2\pi)^{-n/2} \int e^{i\lambda \cdot x} \hat{T}(\lambda)\, d\lambda$$

and

$$\mathbf{S}(x) = (2\pi)^{-n/2} \int e^{i\lambda \cdot x} (i\lambda) \hat{T}(\lambda)\, d\lambda$$

are continuous $\mathbb{R}$- and $\mathbb{R}^n$-valued functions respectively. Moreover, by the dominated convergence theorem

$$\frac{T(x+h) - T(x) - h \cdot \mathbf{S}(x)}{|h|}$$

$$= (2\pi)^{-n/2} \int \left[\frac{e^{i\lambda \cdot (x+h)} - e^{i\lambda \cdot x} - i\lambda \cdot h\, e^{i\lambda \cdot x}}{|h|} \right] \hat{T}(\lambda)\, d\lambda$$

converges to zero as $|h| \downarrow 0$. Thus T is C^1 with $\mathbf{D}T = \mathbf{S}$. Using the fact that $(1 + |\lambda|^\ell)\hat{T} \in L^1(\mathbb{R}^n)$, we repeat this process ℓ times to conclude that $T(x)$ is ℓ times continuously differentiable.

We now treat the general case. Let η and ψ be in $C_0^\infty(\Omega)$ and suppose that both η and ψ equal one in a neighborhood N of a point $x \in \Omega$. Since $T \in W_m(\Omega)$, ψT and ηT are C^ℓ functions on $\mathbb{R}^n$. Furthermore we must have $(\psi T)(x) = (\eta T)(x)$ since otherwise we could find a φ with support in N so that $T(\varphi) = (\psi T)(\varphi) \neq (\eta T)(\varphi) = T(\varphi)$. Thus we can define a function $F(x) = (\psi T)(x)$ on Ω by letting ψ be any $C_0^\infty(\Omega)$ function that is one in a neighborhood of x. By what we proved above, $F(x)$ is ℓ times continuously differentiable.

We complete the proof by showing that in Ω, T is given by $F(x)$. Suppose $\varphi \in C_0^\infty(\Omega)$ and let $\alpha(x)$ be a function in $C_0^\infty(\Omega)$ which equals one on $\overline{\text{supp } \varphi}$. Then

$$T(\varphi) = T(\alpha\varphi) = (\alpha T)(\varphi) = \int_\Omega F(x)\varphi(x)\, dx \quad \blacksquare$$

Sobolev's lemma has extensions to various L^p spaces and under certain conditions to the case where $\ell = m - (n/2)$. These extensions are more difficult to prove and are discussed in the Notes.

Theorem IX.25 (Weyl's lemma) Let u be a weak solution of the equation $-\Delta u = g$ on $\mathbb{R}^n$. If g is a C^m function on an open set $\Omega \subset \mathbb{R}^n$, then on Ω, u is equal to a C^ℓ function for each $\ell \in I_+$ satisfying $\ell < m - (n/2) + 2$. In particular if g is C^∞ in Ω, then u is C^∞ in Ω.

Proof We may assume, without loss of generality, that Ω is bounded. Since $\varphi g \in W_m$ for each $\varphi \in C_0^\infty(\Omega)$, $g \in W_m(\Omega)$. By Theorem IX.23, $u \in W_k(\Omega)$ for some k since $u \in \mathscr{D}'(\mathbb{R}^n)$. If $k < m + 2$, then, using the facts that $u \in W_k(\Omega)$, $-\Delta u = g \in W_k(\Omega)$, and the lemma, we conclude that $u \in W_{k+2}(\Omega)$. Repeating this process we obtain the result that $u \in W_{m+2}(\Omega)$ which implies by Sobolev's lemma that u is a C^ℓ function on Ω for $\ell < m - (n/2) + 2$. ∎

Theorem IX.26 (local regularity for Schrödinger's equation) Let u be a weak solution of the equation $(-\Delta + V)u = Eu$ where V is a measurable function and E is a complex number. Then, if V is equal to a C^∞ function in an open region Ω, u is C^∞ in that region also.

Proof Without loss we may suppose that Ω is bounded. Since $u \in \mathscr{D}'(\mathbb{R}^n)$, $u \in W_k(\Omega)$ for some k by Proposition 3. But, since V is C^∞, $Vu \in W_k(\Omega)$ by Proposition 2. Thus, $u \in W_k(\Omega)$ and $-\Delta u \in W_k(\Omega)$, so by the lemma, $u \in W_{k+2}(\Omega)$. By repeatedly using the lemma we find that $u \in \bigcap_{k=-\infty}^{\infty} W_k(\Omega)$ which implies by Sobolev's lemma that u is C^∞ in Ω. ∎

We remark that our method of proof of Theorem IX.26 can be extended to show that if $V \in C^m(\Omega)$, then $u \in C^\ell(\Omega)$ if $\ell < m - (n/2) + 2$ (Problem 45).

IX.7 The free Hamiltonian for nonrelativistic quantum mechanics

In this section we study $-\Delta$ as an operator on $L^2(\mathbb{R}^n)$. There are two reasonable domains to choose for $-\Delta$,

$$D_{\max} = \{\varphi \mid \varphi \in L^2(\mathbb{R}^n) \text{ and } \Delta\varphi \in L^2(\mathbb{R}^n) \text{ in the sense of distributions}\}$$

$$D_{\min} = C_0^\infty(\mathbb{R}^n)$$

We denote $-\Delta \restriction D_{\max}$ by $T_{\max}$ and $-\Delta \restriction D_{\min}$ by $T_{\min}$.

Theorem IX.27

(a) $\varphi \in D_{\max}$ if and only if $|\lambda|^2\hat{\varphi}(\lambda) \in L^2(\mathbb{R}^n)$ and in that case $T_{\max}\varphi = \widehat{|\lambda|^2\hat{\varphi}(\lambda)}$.

(b) $T_{\max}$ is self-adjoint.

(c) $T_{\min}$ is essentially self-adjoint and $\overline{T}_{\min} = T_{\max}$.

Proof (a) follows immediately from the formula $-\widehat{\Delta T} = |\lambda|^2 \hat{T}$ which is valid for arbitrary tempered distributions. By Proposition 1 of Section VIII.3, multiplication by $|\lambda|^2$ is self-adjoint on $\{\varphi \in L^2(\mathbb{R}^n) \mid |\lambda|^2\varphi \in L^2(\mathbb{R}^n)\}$. Since $\mathscr{F}$ is unitary and $T_{\max} = \mathscr{F}^{-1}|\lambda|^2\mathscr{F}$, $T_{\max}$ is self-adjoint on $D_{\max}$.

To prove that $T_{\min}$ is essentially self-adjoint it is sufficient to show that $T^*_{\min} = T_{\max}$ since then $\overline{T}_{\min} = T^{**}_{\min} = T_{\max}$. Suppose that $\psi \in D(T^*_{\min})$. Then $(-\Delta\varphi, \psi) = (T_{\min}\varphi, \psi) = (\varphi, T^*_{\min}\psi)$ for all $\varphi \in C_0^\infty(\mathbb{R}^n)$. Thus $-\Delta\psi \in L^2(\mathbb{R}^n)$ in the sense of distributions, so $\psi \in D_{\max}$ and $T^*_{\min}\psi = -\Delta\psi = T_{\max}\psi$. Conversely, suppose that $\psi \in D_{\max}$. Then $-\Delta\psi \in L^2(\mathbb{R}^n)$ so that for all $\varphi \in C_0^\infty$, $(-\Delta\varphi, \psi) = (\varphi, -\Delta\psi)$. Thus, $\psi \in D(T^*_{\min})$ and $T^*_{\min}\psi = -\Delta\psi$. ∎

Definition We denote $-\Delta$ with the domain $D_{\max}$ by H_0 and call it the **free Hamiltonian.**

In the remainder of this section we use the Fourier transform and the estimates in Section IX.4 to study various properties of H_0. First we prove a theorem that gives further properties of the functions in $D(H_0)$. Then we derive explicit formulas for $R_\lambda(H_0)$ and e^{itH_0}. Finally, we prove some asymptotic properties of e^{itH_0} which will be useful when we treat scattering theory in Chapter XII.

Since H_0 is self-adjoint, its powers H_0^m are also self-adjoint. Since $H_0^m = \mathscr{F}^{-1}|\lambda|^{2m}\mathscr{F}$, the domain of H_0^m is just the Sobolev space W_{2m} introduced in Section IX.6. Sobolev's lemma (Theorem IX.24) immediately implies:

Proposition A vector $\varphi \in L^2(\mathbb{R}^n)$ is in $C^\infty(H_0) = \bigcap_{m=1}^\infty D(H_0^m)$ if and only if $\varphi \in C^\infty(\mathbb{R}^n)$ and $D^\alpha\varphi \in L^2(\mathbb{R}^n)$ for each α.

More importantly, the vectors in $D(H_0)$ itself have the following properties:

Theorem IX.28 Let $\varphi \in L^2(\mathbb{R}^n)$ be in $D(H_0)$. Then

(a) If $n \leq 3$, φ is a bounded continuous function and for any $a > 0$, there is a b, independent of φ, so that

$$\|\varphi\|_\infty \leq a\|H_0\varphi\| + b\|\varphi\| \tag{IX.25}$$

(b) If $n \geq 4$ and $2 \leq q < 2n/(n-4)$, then $\varphi \in L^q(\mathbb{R}^n)$ and for any $a > 0$ there is a b (depending only on q, n, and a) so that

$$\|\varphi\|_q \leq a\|H_0\varphi\| + b\|\varphi\| \tag{IX.26}$$

Proof By the Riemann–Lebesgue lemma and the Plancherel theorem, (a) will follow if we can prove that $\hat{\varphi} \in L^1(\mathbb{R}^n)$ and

$$\|\hat{\varphi}\|_1 \leq a\|\lambda^2\hat{\varphi}\|_2 + b\|\hat{\varphi}\|_2 \tag{IX.27}$$

We will prove (IX.27) in the case $n = 3$. Suppose $\varphi \in D(H_0)$, then $(1 + \lambda^2)\hat{\varphi}$ and $(1 + \lambda^2)^{-1}$ are in $L^2(\mathbb{R}^3)$ so $\hat{\varphi} \in L^1(\mathbb{R}^3)$ and by the Schwarz inequality

$$\|\hat{\varphi}\|_1 \leq c\|(\lambda^2 + 1)\hat{\varphi}\|_2 \leq c(\|\lambda^2\hat{\varphi}\|_2 + \|\hat{\varphi}\|_2) \tag{IX.28}$$

where $c^2 = \int (1 + \lambda^2)^{-2}\, d\lambda$. For any $r > 0$, let $\hat{\varphi}_r(\lambda) = r^3\hat{\varphi}(r\lambda)$. Then $\|\hat{\varphi}_r\|_1 = \|\hat{\varphi}\|_1$, $\|\hat{\varphi}_r\|_2 = r^{3/2}\|\hat{\varphi}\|_2$, and $\|\lambda^2\hat{\varphi}_r\|_2 = r^{-1/2}\|\lambda^2\hat{\varphi}\|_2$. Thus, using (IX.28) for $\hat{\varphi}_r$, and using these equalities, we obtain

$$\|\hat{\varphi}\|_1 \leq cr^{-1/2}\|\lambda^2\hat{\varphi}\|_2 + cr^{3/2}\|\hat{\varphi}\|_2$$

for any $r > 0$. If we choose r large enough, (IX.27) follows.

By the Hausdorff–Young inequality and the Plancherel theorem, in order to prove (b) we need only show that for any p satisfying $2n/(n + 4) < p \leq 2$ and $a > 0$ there is a b so that

$$\|\hat{\varphi}\|_p \leq a\|\lambda^2\hat{\varphi}\|_2 + b\|\hat{\varphi}\|_2$$

The Hölder inequality implies that

$$\|\hat{\varphi}\|_p^p \leq \|(1 + \lambda^2)^{-p}\|_r \|(1 + \lambda^2)^p|\hat{\varphi}|^p\|_s$$

where $r^{-1} + s^{-1} = 1$. Choosing $s = 2/p$, the triangle inequality shows that

$$\begin{aligned}\|(1 + \lambda^2)^p|\hat{\varphi}|^p\|_s &= (\|(1 + \lambda^2)|\hat{\varphi}|\,\|_2)^p \\ &\leq (\|\hat{\varphi}\|_2 + \|\lambda^2\hat{\varphi}\|_2)^p\end{aligned}$$

Thus if $\|(1 + \lambda^2)^{-p}\|_{2(2-p)^{-1}} = c_1 < \infty$, we have

$$\|\hat{\varphi}\|_p \leq c_1^{1/p}(\|\lambda^2\hat{\varphi}\|_2 + \|\hat{\varphi}\|_2)$$

But

$$\|(1 + \lambda^2)^{-p}\|_{2(2-p)^{-1}}^{2(2-p)^{-1}} = \int \frac{d\lambda}{(1 + \lambda^2)^{2p(2-p)^{-1}}} < \infty$$

if $4p(2 - p)^{-1} > n$, i.e. if $p > 2n/(4 + n)$. The method of proving that the constant in front of $\|\lambda^2\hat{\varphi}\|$ can be chosen arbitrarily small is the same as in part (a). ∎

We will see in Section X.2 that part (b) of the theorem holds in the case $n \geq 5$ and $q = 2n/(n - 4)$ for some fixed a.

We turn now to computing explicit formulas for $(H_0 - E)^{-1}$, $E \in \mathbb{C}\backslash[0, \infty)$, and $e^{-iH_0 t}$, $\operatorname{Im} t \leq 0$. Since $H_0 = \mathscr{F}^{-1}\lambda^2\mathscr{F}$, $f(H_0) = \mathscr{F}^{-1}f(\lambda^2)\mathscr{F}$ where f is any bounded measurable function. That is, both $(H_0 - E)^{-1}$ and $e^{-iH_0 t}$ can be expressed in terms of multiplication operators:

$$(H_0 - E)^{-1} = \mathscr{F}^{-1}(\lambda^2 - E)^{-1}\mathscr{F}; \qquad e^{-iH_0 t} = \mathscr{F}^{-1}e^{-i\lambda^2 t}\mathscr{F}$$

Since the Fourier transform takes multiplication into convolution, we will get simple expressions for $(H_0 - E)^{-1}$ and $e^{-iH_0 t}$ as convolution operators.

Let $f \in L^\infty(\mathbb{R}^n)$; we denote the operator $\varphi \mapsto \widetilde{(f\hat{\varphi})}$ on $L^2(\mathbb{R}^n)$ by $f(-i\nabla)$. Notice that $f(-i\nabla)$ is a well-defined bounded operator since multiplication by f is bounded.

Theorem IX.29 Let $f \in L^\infty(\mathbb{R}^n)$. If either (i) $f \in L^2(\mathbb{R}^n)$ *or* (ii) $\check{f} \in L^1(\mathbb{R}^n)$, then

$$(f(-i\nabla)\varphi)(x) = (2\pi)^{-n/2}\int \check{f}(x - y)\varphi(y)\, dy \tag{IX.29}$$

for all $\varphi \in L^2(\mathbb{R}^n)$. The integral converges for all x in case (i) and for almost all x in case (ii).

Proof Suppose $f \in L^2 \cap L^\infty$ and $\varphi \in \mathscr{S}$. Then $f \in \mathscr{S}'$ so by Theorem IX.4,

$$\begin{aligned} f(-i\nabla)\varphi \equiv \widetilde{(f\hat{\varphi})} &= (2\pi)^{-n/2}\check{f} * \varphi \\ &= (2\pi)^{-n/2}\int \check{f}(y)\varphi(x - y)\, dy \end{aligned}$$

so (IX.29) holds if $\varphi \in \mathscr{S}$. For $\varphi \in L^2(\mathbb{R}^n)$, we can find a sequence $\varphi_m \in \mathscr{S}$ so that $\varphi_m \xrightarrow{L^2} \varphi$. Since $f \in L^\infty$, $f\hat{\varphi}_m \xrightarrow{L^2} f\hat{\varphi}$, so $f(-i\nabla)\varphi_m \to f(-i\nabla)\varphi$. Thus we can find a subsequence (which we also call $\{\varphi_m\}$) so that $f(-i\nabla)\varphi_m \to f(-i\nabla)\varphi$ pointwise a.e. Since $\check{f} \in L^2(\mathbb{R}^n)$,

$$\begin{aligned} \lim_{m\to\infty}(f(-i\nabla)\varphi_m)(x) &= \lim_{m\to\infty}(2\pi)^{-n/2}\int \check{f}(x - y)\varphi_m(y)\, dy \\ &= (2\pi)^{-n/2}\int \check{f}(x - y)\varphi(y)\, dy \end{aligned}$$

for each $x \in \mathbb{R}^n$. We have thus proven IX.29 in case (i).

To prove (IX.29) in case (ii), observe that if f_m and φ are in $\mathscr{S}(\mathbb{R}^n)$, then

$f_m(-i\nabla)\varphi = (2\pi)^{-n/2}\check{f}_m * \varphi$. Choose $f_m \in \mathscr{S}(\mathbb{R}^n)$ so that $\check{f}_m \xrightarrow{L^1} \check{f}$. Then $f_m \xrightarrow{L^2} f$, so $f_m\hat{\varphi} \xrightarrow{L^2} f\hat{\varphi}$. Thus

$$\begin{aligned} f(-i\nabla)\varphi &= \lim_{m\to\infty} (2\pi)^{-n/2}\check{f}_m * \varphi \\ &= (2\pi)^{-n/2}\check{f} * \varphi \end{aligned}$$

by Young's inequality. Since the bounded operators, $f(-i\nabla)$ and convolution by $(2\pi)^{-n/2}\check{f}$ agree on $\mathscr{S}$, they agree on all of $L^2(\mathbb{R}^n)$. That the convolution, $\check{f} * \varphi$, is given by an absolutely convergent integral is proven in Example 1 of Section IX.4. ∎

Example 1 (the free resolvent, $n = 3$) Let $E = -\kappa^2$, where $\operatorname{Re}\kappa > 0$. Thus $E \in \rho(H_0)$. Since $f(\lambda) \equiv (\lambda^2 + \kappa^2)^{-1} \in L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, we can use part (i) of Theorem IX.29 to compute $(H_0 - E)^{-1}$. Since $f \in L^2$,

$$(2\pi)^{-3/2}\check{f}(x) = \underset{R\to\infty}{\text{l.i.m.}}(2\pi)^{-3}\int_{|\lambda|\le R} \frac{e^{i\lambda\cdot x}}{\lambda^2 + \kappa^2}\, d\lambda$$

Changing to spherical coordinates, set $u = \cos\sigma = \lambda \cdot x/|x||\lambda|$ and $r = |\lambda|$. Then

$$\begin{aligned} (2\pi)^{-3/2}\check{f}(x) &= \underset{R\to\infty}{\text{l.i.m.}}(2\pi)^{-2}\int_0^R \int_{-1}^1 \frac{e^{ir|x|u}}{r^2 + \kappa^2}\, r^2\, dr\, du \\ &= \underset{R\to\infty}{\text{l.i.m.}} \frac{(2\pi)^{-2}}{i|x|}\int_{-R}^R \frac{e^{ir|x|}r}{r^2 + \kappa^2}\, dr \\ &= \underset{R\to\infty}{\text{l.i.m.}} \frac{(2\pi)^{-2}}{i|x|}\int_{C_R} \frac{\tilde{r}e^{i\tilde{r}|x|}}{(\tilde{r} + i\kappa)(\tilde{r} - i\kappa)}\, d\tilde{r} \end{aligned}$$

where $\tilde{r}$ is in the complex r plane and C_R is the curve shown in

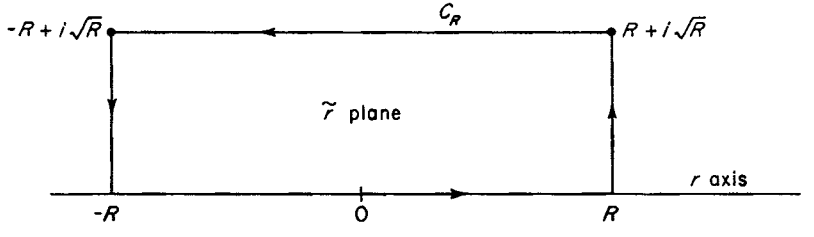


FIGURE IX.5 The path C_R.

Figure IX.5. For each $|x|$ the limit exists and equals $e^{-\kappa|x|}/4\pi|x|$. Thus, from Theorem IX.29 we have

$$(n = 3) \qquad [(H_0 + \kappa^2)^{-1}\varphi](x) = (4\pi)^{-1} \int \frac{e^{-\kappa|x-y|}}{|x-y|} \varphi(y)\, dy \qquad \text{(IX.30)}$$

The function $G_0(x, y; E) = e^{-\kappa|x-y|}/4\pi|x-y|$ is often called the **free Green's function.**

Example 2 (the free resolvent, $n \neq 3$) If n does not equal one or three, the computation of the inverse Fourier Transform of $(\lambda^2 + \kappa^2)^{-1}$ is not as explicit as in Example 1; it turns out to be an expression in terms of Bessel functions. It is not hard to see, however, that if $f(\lambda) = (\lambda^2 + \kappa^2)^{-1}$, then $\check{f} \in L^1(\mathbb{R}^n)$ (see Example 6 in Section IX.10 and Problem 49). Thus, we are in case (ii) of Theorem IX.29. Additional properties of Green's functions are given in Problem 49.

Example 3 (the free propagator) We want to compute an explicit formula for e^{-iH_0t}, $t \in \mathbb{R}$, the unitary group which gives the free quantum dynamics. $e^{-i\lambda^2 t}$ does not satisfy either of the criteria in Theorem IX.29 so we proceed as follows: Suppose that $\alpha \in \mathbb{C}$ and $\operatorname{Re}\alpha > 0$. Then

$$e^{-\lambda^2\alpha} \in L^2(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$$

so

$$(e^{-H_0\alpha}\varphi)(x) = \left(\frac{1}{4\pi\alpha}\right)^{n/2} \int e^{-|x-y|^2/4\alpha}\varphi(y)\, dy$$

since $\mathscr{F}^{-1}(e^{-\lambda^2\alpha}) = (2\alpha)^{-n/2}e^{-x^2/4\alpha}$ (Example 1 of Section IX.1). Now, suppose that $\varphi \in L^1 \cap L^2$. Since $e^{-i(t-i\varepsilon)H_0}\varphi \xrightarrow{L^2} e^{-itH_0}\varphi$ as $\varepsilon \downarrow 0$, we can find a subsequence which converges pointwise a.e. Thus

$$\begin{aligned}(e^{-itH_0}\varphi)(x) &= \lim_{\varepsilon \downarrow 0} (e^{-i(t-i\varepsilon)H_0}\varphi)(x) \\ &= \lim_{\varepsilon \downarrow 0} (4\pi i(t - i\varepsilon))^{-n/2} \int e^{-|x-y|^2/4i(t-i\varepsilon)}\varphi(y)\, dy \\ &= (4\pi i t)^{-n/2} \int e^{i|x-y|^2/4t}\varphi(y)\, dy\end{aligned}$$

by the dominated convergence theorem. For general $\varphi \in L^2(\mathbb{R}^n)$, we can now use the trick employed in Section IX.2 to conclude that

$$(e^{-itH_0}\varphi)(x) = \text{l.i.m.}(4\pi i t)^{-n/2} \int e^{i|x-y|^2/4t}\varphi(y)\, dy \qquad \text{(IX.31)}$$

The function $P_0(x, y; t) = (4\pi it)^{-n/2} e^{i|x-y|/4t}$ is often called the **free propagator**.

To show how useful these explicit formulas are, we will derive two consequences of (IX.31) which are useful in scattering theory. The first is an estimate reflecting the spreading of free wave packets.

Theorem IX.30 Let H_0 be the free Hamiltonian on $\mathbb{R}^n$. Let $2 \leq q \leq \infty$ and $p = (1 - q^{-1})^{-1}$. Then

$$\|e^{-itH_0}\varphi\|_q \leq t^{-n(p^{-1}-1/2)}\|\varphi\|_p \tag{IX.32}$$

Proof Since e^{-itH_0} is unitary on $L^2(\mathbb{R}^n)$, $\|e^{-itH_0}\varphi\|_2 = \|\varphi\|_2$. If $\varphi \in L^1 \cap L^2$, then it follows from (IX.31) that $\|e^{-itH_0}\varphi\|_\infty \leq (4\pi t)^{-n/2}\|\varphi\|_1$. By the Riesz–Thorin theorem, e^{-itH_0} extends uniquely to a map from $L^p(\mathbb{R}^n)$ to $L^q(\mathbb{R}^n)$ and the estimate (IX.32) holds. ∎

The second application of (IX.31) is to prove an explicit asymptotic formula for e^{-itH_0}.

Theorem IX.31 Let H_0 be the free Hamiltonian on $\mathbb{R}^n$ and suppose $\varphi \in L^2(\mathbb{R}^n)$. Then

$$(e^{-itH_0}\varphi)(x) \to (2it)^{-n/2} e^{ix^2/4t}\hat{\varphi}(x/2t) \tag{IX.33}$$

in the sense that the difference goes to zero in L^2-norm as $t \to \infty$.

Proof For fixed t, the map V_t: $\varphi \to (2it)^{-n/2} e^{ix^2/4t}\hat{\varphi}(x/2t)$ is unitary so we need only prove the statement of the theorem for $\varphi \in \mathscr{S}$ and then use an $\varepsilon/3$ argument. Since

$$e^{i|x-y|^2/4t} = e^{ix^2/4t} e^{-ix\cdot y/2t} e^{iy^2/4t}$$

from (IX.31) we have

$$(e^{-iH_0 t}\varphi)(x) - (V_t\varphi)(x) = (4\pi it)^{-n/2} e^{ix^2/4t} \int (e^{iy^2/4t} - 1) e^{-ix\cdot y/2t}\varphi(y)\, dy$$

$$= \frac{e^{ix^2/4t}}{(2it)^{n/2}}\, \hat{G}_t\left(\frac{x}{2t}\right)$$

where $G_t(y) = (e^{iy^2/4t} - 1)\varphi(y)$. Thus

$$\begin{aligned}\|e^{-iH_0t}\varphi - V_t\varphi\|_2 &= (2t)^{-n/2}\|\hat{G}_t(\cdot/2t)\|_2 \\ &= \|\hat{G}_t(\cdot)\|_2 \\ &= \|G_t\|_2 \\ &\leq \frac{1}{4t}\|y^2\varphi(y)\|_2 \\ &\to 0 \qquad \text{as} \quad t \to \infty\end{aligned}$$

In the last step we used the estimate

$$|e^{iy^2/4t} - 1| = \left|\int_0^{y^2/4t} \frac{d}{dx}(e^{ix})\,dx\right| \leq \frac{y^2}{4t} \quad \blacksquare$$

Formula (IX.33) has a simple physical interpretation. To see this, we reintroduce the mass m by taking $H_0 = (-1/2m)\,\Delta$. If the system is in state φ at $t = 0$, then by (IX.33) the asymptotic probability density for position is $(m/t)^n|\hat{\varphi}(mx/t)|^2$. But $|\hat{\varphi}(\lambda)|^2$ is the initial probability density for momentum. Thus, for large times, the probability of a particle being at x at time t is proportional to the probability of its having momentum mx/t initially. So, for large times, the quantum free particle behaves like a classical free particle starting at $x = 0$ at time $t = 0$ with momentum density $|\hat{\varphi}(\lambda)|^2$.

IX.8 The Gårding–Wightman axioms

In this section we discuss several applications of the Fourier transform to the theory of quantized fields. It is not necessary for the reader to have had any previous experience with quantum field theory. We begin with a brief history, state the Wightman axioms, and define the Wightman functions. Then we use the Fourier transform to prove analyticity properties of the Wightman functions, outline the proof of the PCT theorem, and derive the Källen–Lehmann representation for the two-point function. In an appendix, we discuss Lorentz invariant measures.

Quantum field theory began in the twenties as an attempt to combine quantum mechanics and special relativity in a quantum generalization of the classical models for electromagnetic phenomena. Since then, field theory

has been used extensively to construct models for many elementary particle phenomena. From the beginning, it was apparent to the founders of the subject (Heisenberg, Pauli, Dirac) that there were many mathematical difficulties in the theory. Nevertheless, field theory continued to grow and by the forties had become a maze of folk theorems, conjectures, and complicated perturbation theory calculations, all difficult to prove since the central objects of the theory, the fields themselves, were only vaguely defined. Despite the fact that the theory lacked sound mathematical foundations, Schwinger, Feynman, Tomonaga, Dyson, and others systematized perturbation theory in the late 1940's to make calculations about electrodynamics. The striking experimental verification of these calculations suggested that within quantum field theory there were sound mathematical models for at least some elementary particle phenomena.

It was in this atmosphere that Gårding and Wightman formulated a definition of "quantum field" by proposing a set of mathematical properties which they argued every quantum field theory should possess. These properties are called **Wightman axioms**. The study of the Wightman axioms and their mathematical consequences is usually called **axiomatic quantum field theory**. This name is somewhat misleading for it has given many people the mistaken impression that the main interest is the axioms themselves rather than their mathematical consequences and the construction of specific examples. For this reason the subject is sometimes called "the general theory of quantized fields."

For simplicity we will only give the axioms for a "Hermitian scalar quantum field theory"; other cases are mentioned in the notes. We use units where the rationalized Planck's constant and the velocity of light are equal to one. Since we discuss each property briefly the definition is rather spread out.

*A **Hermitian scalar quantum field theory** is a quadruple $\langle \mathscr{H}, U, \varphi, D \rangle$ which satisfies the following properties* (1–8):

Property 1 (***relativistic invariance of states***) *$\mathscr{H}$ is a separable Hilbert space and $U(\cdot, \cdot)$ is a strongly continuous unitary representation on $\mathscr{H}$ of the restricted Poincaré group.*

The restricted Poincaré group is defined as follows: Let $x = \langle x^0, x^1, x^2, x^3 \rangle$ and $y = \langle y^0, y^1, y^2, y^3 \rangle$ be two vectors in $\mathbb{R}^4$. The Lorentz scalar product of x and y is defined to be $x^0y^0 - x^1y^1 - x^2y^2 - x^3y^3$. x^0 is called the time component of x; $\langle x^1, x^2, x^3 \rangle$ is called the space

component. We denote by x_μ the components of the vector $\tilde{x} = (x^0, -x^1, -x^2, -x^3)$ so the Lorentz scalar product of x and y is just the usual inner product of x and $\tilde{y}$. Using the Einstein convention we will sometimes write the sum $\sum_{\mu=0}^{3} x^\mu y_\mu$ simply as $x^\mu y_\mu$, the summation being understood. The **Lorentz group** $\mathscr{L}$ is the set of linear transformations on $\mathbb{R}^4$ that preserve the Lorentz scalar product. The **restricted Lorentz group** $\mathscr{L}_+^\uparrow$ is the subgroup of those $\Lambda \in \mathscr{L}$ with $\det \Lambda = 1$ and with the matrix element between $\langle 1, 0, 0, 0\rangle$ and itself positive. The **restricted Poincaré group** $\mathscr{P}_+^\uparrow$, is the set of pairs $\langle a, \Lambda\rangle$ where $a \in \mathbb{R}^4$ and $\Lambda \in \mathscr{L}_+^\uparrow$ with the group operation

$$\langle a, \Lambda_1\rangle\langle b, \Lambda_2\rangle = \langle a + \Lambda_1 b, \Lambda_1\Lambda_2\rangle$$

$\mathscr{P}_+^\uparrow$ acts naturally on $\mathbb{R}^4$ by $\langle a, \Lambda\rangle x = \Lambda x + a$ and is sometimes called the family of relativistic transformations of $\mathbb{R}^4$.

If we fix $\Lambda = I$, then $U(a) = U(a, I)$ is a strongly continuous unitary representation of $\mathbb{R}^4$. From Theorem VIII.12 if follows that there are four commuting self-adjoint operators P_0, P_1, P_2, P_3 on $\mathscr{H}$ and a projection-valued measure E_Ω on $\mathbb{R}^4$ so that

$$(\varphi, U(a)\varphi) = (\varphi, \exp(ia^\mu P_\mu)\varphi) = \int_{\mathbb{R}^4} e^{ia^\mu\lambda_\mu}\, d(\varphi, E_\lambda \varphi) \qquad \text{(IX.34)}$$

P_0 is called the **Hamiltonian** (or energy operator); P_j, $j = 1, 2, 3$, are the **momentum** operators.

Property 2 (*spectral condition*) *The projection-valued measure E_Ω on $\mathbb{R}^4$ corresponding to $U(a, I) = e^{ia^\mu P_\mu}$ has support in the closed forward light cone.*

The closed forward light cone is the set $\bar{V}_+ = \{x \mid x \cdot \tilde{x} \geq 0,\ x^0 \geq 0\}$. Its interior will be denoted by V_+. The spectral condition is equivalent to the condition that the operators P_0 and $P_0^2 - P_1^2 - P_2^2 - P_3^2$ are both positive.

Property 3 (*existence and uniqueness of the vacuum*) *There exists a unique vector $\psi_0 \in \mathscr{H}$ so that $U(a, I)\psi_0 = \psi_0$ for all $a \in \mathbb{R}^4$. ψ_0 is called the vacuum.*

Property 3 implies that the point $\langle 0, 0, 0, 0\rangle$ has nonzero E_Ω-measure and that $E_{\langle 0,0,0,0\rangle}$ has a one-dimensional range. The $U(0, \Lambda)$ leave Ran $E_{\langle 0,0,0,0\rangle}$ invariant so $U(0, \Lambda) \restriction \text{Ran } E_{\langle 0,0,0,0\rangle}$ is a one-dimensional representation of $\mathscr{L}_+^\uparrow$. Since the only one-dimensional representation of $\mathscr{L}_+^\uparrow$ is the identity representation, it follows that $U(a, \Lambda)\psi_0 = \psi_0$ for all $\langle a, \Lambda\rangle \in \mathscr{P}_+^\uparrow$.

Property 4 (*invariant domains for fields*) *There is a dense subspace* $D \subset \mathscr{H}$ *and a map* φ *from* $\mathscr{S}(\mathbb{R}^4)$ *to the (unbounded) operators on* $\mathscr{H}$ *so that*

(i) For each $f \in \mathscr{S}(\mathbb{R}^4)$, $D \subset D(\varphi(f))$, $D \subset D(\varphi(f)^*)$ and $\varphi(f)^* \restriction D = \varphi(\bar{f}) \restriction D$.
(ii) $\psi_0 \in D$ and $\varphi(f)D \subset D$ for all $f \in \mathscr{S}(\mathbb{R}^4)$.
(iii) For fixed $\psi \in D$, the map $f \mapsto \varphi(f)\psi$ is linear.

Early formulations of field theory treated φ as an operator-valued function though the founders of the subject were aware that $\varphi(x)$ was a very singular object. The operator $\varphi(x)$ was said to be the "field at the point x" analogously to the classical electromagnetic field. This formulation led to various difficulties which were overcome by taking the field φ to be an operator-valued distribution rather than an operator-valued function; i.e., φ is defined on $\mathscr{S}(\mathbb{R}^4)$ rather than on $\mathbb{R}^4$. $\varphi(f)$ should be thought of as the space–time average of the hypothetical $\varphi(x)$ with the averaging function f. Symbolically

$$\varphi(f) = \int_{\mathbb{R}^4} \varphi(x) f(x)\, dx.$$

Bohr and Rosenfeld pointed out that from a physical point of view it is impossible to measure the electric field strength at a point because of certain quantum-mechanical effects related to the uncertainty principle. So, from a mathematical and a *physical* point of view it is reasonable to consider the **smeared field** $\varphi(f)$. In fact, it can be shown (Problem 53) that in a quantum field theory satisfying Properties 1–8, the field $\varphi(f)$ cannot arise from integrating a well-defined operator-valued function $\varphi(x)$ against $f(x)$.

The choice of $\mathscr{S}(\mathbb{R}^4)$ as a test function space for $\varphi(\cdot)$, rather than $C_0^\infty(\mathbb{R}^4)$ or some other test function space, is not absolutely necessary. Jaffe has made a detailed study of this question (see the Notes). The reason that we require (ii) is so that the **vacuum expectation values** $(\psi_0, \varphi(f_1) \cdots \varphi(f_n)\psi_0)$ make sense. One might suppose that it would be more useful to assume that $\varphi(f)$ is essentially self-adjoint on D rather than just symmetric, but this extra assumption seems to have few consequences.

Property 5 (*regularity of the field*) *For any* ψ_1 *and* ψ_2 *in* D, *the map* $f \mapsto (\psi_1, \varphi(f)\psi_2)$ *is a tempered distribution.*

The stronger statement that for $\psi \in D$, $f \mapsto \varphi(f)\psi$ is strongly continuous is a consequence of Properties 4 and 5 (Problem 54).

Property 6 (*Poincaré invariance of the field*) *For each* $\langle a, \Lambda \rangle \in \mathscr{P}_+^\uparrow$, $U(a, \Lambda)D \subset D$ *and for all* $f \in \mathscr{S}(\mathbb{R}^4)$, $\psi \in D$,

$$U(a, \Lambda)\varphi(f)U(a, \Lambda)^{-1}\psi = \varphi(\langle a, \Lambda \rangle f)\psi$$

where

$$\langle a, \Lambda \rangle f(x) = f(\Lambda^{-1}(x - a))$$

The invariance condition is often written formally as

$$U(a, \Lambda)\varphi(x)U(a, \Lambda)^{-1} = \varphi(\Lambda x + a)$$

Property 7 (*local commutativity or microscopic causality*) *If* f *and* g *in* $\mathscr{S}(\mathbb{R}^4)$ *have supports which are spacelike separated, then*

$$[\varphi(f)\varphi(g) - \varphi(g)\varphi(f)]\psi = 0$$

for all $\psi \in D$.

Two sets $S_1, S_2 \subset \mathbb{R}^4$ are called **spacelike separated** if $x \in S_1$ and $y \in S_2$ implies that $(x - y) \cdot \widetilde{(x - y)} < 0$. Property 7 expresses mathematically the quantum-mechanical statement that measurements in spacelike separated regions should not interfere with each other.

Property 8 (*cyclicity of the vacuum*) *The set* D_0 *of finite linear combinations of vectors of the form* $\varphi(f_1) \cdots \varphi(f_n)\psi_0$ *is dense in* $\mathscr{H}$.

This property ensures that the Hilbert space $\mathscr{H}$ is not too large, or put another way that the theory can be described in terms of a single field φ.

This completes the definition of a Hermitian scalar quantum field theory. There are two ways in which a mathematical investigation can now proceed. First, one can investigate the consequences of these axioms. The main bulk of the work in axiomatic field theory in the fifties and early sixties was of this type. In the remainder of this section we will show how the Fourier transform is used in deriving consequences of the axioms. The second general problem is to construct models satisfying all (or at least some) of the axioms. It was known when the axioms were formulated that they were consistent since the theory of free fields (see Section X.7) satisfies all the properties. Unfortunately, free field theories describe systems of particles that do not interact. It has proven very difficult to construct interesting

(i.e. interacting) examples. Some progress has been made on this problem in recent years (see Section X.7 and Chapter XIX).

We begin our discussion of the consequences of the axioms by defining the functionals

$$\mathscr{W}_n(f_1, \ldots, f_n) = (\psi_0, \varphi(f_1) \cdots \varphi(f_n)\psi_0)$$

The $\{\mathscr{W}_n\}$ are called **Wightman functions** or **Wightman distributions** or **vacuum expectation values**; $\mathscr{W}_n$ is sometimes called the ***n*-point function**. We will see in Chapter XVII that a field theory can be recovered from a knowledge of its Wightman functions. Let $\psi_1 = \varphi(\overline{f}_{k-1}) \cdots \varphi(\overline{f}_1)\psi_0$ and $\psi_2 = \varphi(f_{k+1}) \cdots \varphi(f_n)\psi_0$. Then by Property 4, ψ_1 and ψ_2 are in D so by Property 5 $\mathscr{W}_n(f_1, \ldots, f_n) = (\psi_1, \varphi(f_k)\psi_2)$ is continuous in f_k when the other f's are held fixed. Thus, $\mathscr{W}_n(f_1, \ldots, f_n)$ is a separately continuous multilinear functional on $\bigtimes_1^n \mathscr{S}(\mathbb{R}^4)$. Thus, by the nuclear theorem (Theorem V.12), there is a distribution $\tilde{\mathscr{W}}_n$ in $\mathscr{S}'(\mathbb{R}^{4n})$ so that $\mathscr{W}_n(f_1, f_2, \ldots, f_n) = \tilde{\mathscr{W}}_n(f_1 f_2 \cdots f_n)$ if $f_i \in \mathscr{S}(\mathbb{R}^4)$. We denote $\tilde{\mathscr{W}}_n$ by $\mathscr{W}_n$ also.

From Properties 3 and 6 it follows that $\mathscr{W}_n$ has the invariance property:

$$\mathscr{W}_n(\langle a, \Lambda\rangle f_1, \ldots, \langle a, \Lambda\rangle f_n) = \mathscr{W}_n(f_1, \ldots, f_n)$$

for all $\langle a, \Lambda\rangle \in \mathscr{P}_+^\uparrow$. In particular,

$$\mathscr{W}_n(f_1(x_1 - a), f_2(x_2 - a), \ldots, f_n(x_n - a)) = \mathscr{W}_n(f_1, \ldots, f_n) \quad \text{(IX.35)}$$

By a simple analysis (see Problem 56), it follows from (IX.35) that there is a distribution $W_n \in \mathscr{S}'(\mathbb{R}^{4n-4})$ so that symbolically

$$\mathscr{W}_n(x_1, \ldots, x_n) = W_n(x_1 - x_2, x_2 - x_3, \ldots, x_{n-1} - x_n)$$

That is, for $f \in \mathscr{S}(\mathbb{R}^{4n})$,

$$\mathscr{W}_n(f) = \int_{\mathbb{R}_4} W_n(f_{(x)})\, dx$$

where

$$f_{(x)}(\xi_1, \ldots, \xi_{n-1}) = f(x, x - \xi_1, x - \xi_1 - \xi_2, \ldots, x - \xi_1 - \cdots - \xi_{n-1})$$

We have already introduced the notation V_+ for the forward light cone and $\overline{V}_+$ for the closed forward light cone. Define

$$V_+^{(n)} = \{\langle x_1, \ldots, x_n\rangle \in \mathbb{R}^{4n} \mid x_i \in V_+ \text{ for each } i\}$$

Note that $V_+^{(n)}$ and its closure $\overline{V}_+^{(n)}$ are cones. Let

$$\mathscr{T}_n = \mathbb{R}^{4n} - iV_+^{(n)}$$

We will call $\mathscr{T}_n$ the **forward tube.**

We are now ready to state and prove an important theorem about the Wightman distributions.

Theorem IX.32 For each $n \geq 1$, $\hat{W}_n$ has support in $-\overline{V_+^{(n-1)}}$ and W_n is the boundary value of a function analytic in the forward tube $\mathcal{T}_{n-1}$.

Proof Let k be given, $1 \leq k \leq n$, and let a be in $\mathbb{R}^4$. Then

$$\begin{aligned}
&\mathcal{W}_n(f_1(x_1)\cdots f_k(x_k)f_{k+1}(x_{k+1}-a)\cdots f_n(x_n-a)) \\
&\quad = (\psi_0, \varphi(f_1)\cdots\varphi(f_k)U(a)\varphi(f_{k+1})\cdots\varphi(f_n)\psi_0) \\
&\quad = \int_{\mathbb{R}^4} e^{i\lambda\cdot\tilde{a}}\, d(\psi_1, E_\lambda\psi_2) \\
&\quad = \int_{\mathbb{R}^4} e^{i\tilde{\lambda}\cdot a}\, d(\psi_1, E_\lambda\psi_2) \\
&\quad = \int_{\mathbb{R}^4} e^{i\lambda\cdot a}\, d(\psi_1, E_{\tilde{\lambda}}\psi_2)
\end{aligned}$$

where $\psi_1 = \varphi(f_k)^*\cdots\varphi(f_1)^*\psi_0$ and $\psi_2 = \varphi(f_{k+1})\cdots\varphi(f_n)\psi_0$. By Property 2, $d(\psi_1, E_\lambda\psi_2)$ has support in $\overline{V_+}$. Since $\lambda \mapsto \tilde{\lambda}$ takes $\overline{V_+}$ into itself, $d(\psi_1, E_{\tilde{\lambda}}\psi_2)$ also has support in $\overline{V_+}$. Now let

$$g(\xi_1, \ldots, \xi_{n-1}) = \prod_{j=2}^{n} f_j\left(-\sum_{i=1}^{j}\xi_i\right)$$

and suppose that $h_k \in \mathcal{S}(\mathbb{R}^4)$ is real-valued. In the following calculation we suppress the arguments $\xi_2, \ldots, \xi_{k-1}, \xi_{k+1}, \ldots, \xi_{n-1}$ of g.

$$\begin{aligned}
&\int_{\mathbb{R}^4} h_k(a)\mathcal{W}_n(f_1(x_1)\cdots f_k(x_k-a)\cdots f_n(x_n-a))\, da \qquad \text{(IX.36)} \\
&\quad = \int_{\mathbb{R}^4}\int_{\mathbb{R}^4} W_n(g(\xi_1 - x_1, \xi_k + a))f_1(x_1)h_k(a)\, dx_1\, da \\
&\quad = W_n\left(\int_{\mathbb{R}^4}\int_{\mathbb{R}^4} g(\xi_1 - x_1, \xi_k + a)f_1(x_1)h_k(a)\, dx_1\, da\right) \\
&\quad = W_n(g * (f_1\tilde{h}_k)) \\
&\quad = (2\pi)^{(n-1)/2}\,\hat{W}_n(\check{g}\check{f}_1\hat{h}_k)
\end{aligned}$$

where $\tilde{h}_k(a) = h_k(-a)$. On the other hand,

$$\begin{aligned}
\text{(IX.36)} &= \int_{\mathbb{R}^4} h_k(a)\int_{\mathbb{R}^4} e^{i\tilde{\lambda}\cdot a}\, d(\psi_1, E_{\tilde{\lambda}}\psi_2)\, da \\
&= (2\pi)^{1/2}\int_{\mathbb{R}^4} \check{h}_k(\lambda)\, d(\psi_1, E_{\tilde{\lambda}}\psi_2)
\end{aligned}$$

Therefore $\hat{W}_n(\check{g}\check{f}_1\hat{h}_k) = 0$ if $(\operatorname{supp} \check{h}_k) \cap V_+ = \varnothing$. Since this is true for each k and since the set of finite linear combinations of such functions $\check{f}_1\check{g}$ is dense in $\mathscr{S}(\mathbb{R}^{4n-4})$, we conclude that the support of $\hat{W}_n$ is contained in $-V_+^{(n-1)}$. The conclusion of the theorem now follows from Theorem IX.16. ∎

Because the cone $V_+^{(n-1)}$ does not have a spherical base (if $n > 2$), we have used the generalization of Theorem X.16 given in Problem 23. The phrase "boundary value" in the statement of the theorem means boundary value in the sense of tempered distributions as explained in Section IX.3. Although we have not stated them explicitly, the estimates of Theorem IX.16 give corresponding estimates on the analytic continuation of the Wightman distributions.

An important use of the analyticity properties is to show that the Wightman functions obey certain symmetry relations. Here is a sketch of a typical argument. For simplicity of notation, we will pretend that the Wightman distributions are functions $W_n(\xi_1, \ldots, \xi_{n-1})$. The reader can easily supply the necessary test functions. Limits are always taken in the sense of $\mathscr{S}'(\mathbb{R}^{4n-4})$.

Because of Property 6,

$$W_n(z_1, \ldots, z_{n-1}) = W_n(\Lambda z_1, \ldots, \Lambda z_{n-1}) \tag{IX.37}$$

for all $z_j = \xi_i - i\eta_j$, $\eta_j \in V_+$ and $\Lambda \in \mathscr{L}_+^\uparrow$. Notice that the right-hand side of (IX.37) makes sense since $\Lambda\colon V_+ \to V_+$. Let $\mathscr{L}_+(\mathbb{C})$ denote the set of *complex* 4×4 matrices, Λ, of determinant one that satisfy $\Lambda z \cdot \widetilde{\Lambda z} = z \cdot \tilde{z}$. $\mathscr{L}_+(\mathbb{C})$ is a six-parameter complex manifold which contains the six-parameter real manifold $\mathscr{L}_+^\uparrow$. An elegant technical result, the Bargmann–Hall–Wightman theorem, states that W_n can be extended to be an analytic function on

$$\mathscr{T}_{n-1}^{e} = \{\langle \Lambda z_1, \ldots, \Lambda z_{n-1}\rangle \,\big|\, \langle z_1, \ldots, z_{n-1}\rangle \in \mathscr{T}_{n-1}, \Lambda \in \mathscr{L}_+(\mathbb{C})\}$$

so that (IX.37) still holds, but Λ is now allowed to range over $\mathscr{L}_+(\mathbb{C})$. $\mathscr{T}_{n-1}^{e}$ is called the **extended forward tube**. $\mathscr{T}_{n-1}^{e}$ contains certain real points called **Jost points**; in fact it can be shown that $\langle \xi_1, \ldots, \xi_{n-1}\rangle \in \mathscr{T}_{n-1}^{e} \cap \mathbb{R}^{4n-4}$ if and only if all vectors of the form $\zeta = \sum_{j=1}^{n-1} \lambda_j \xi_j$, with $\lambda_j \geq 0$ and $\sum \lambda_j > 0$, are spacelike, that is, $\xi \cdot \tilde{\xi} < 0$. Thus if $\langle x_1 - x_2, x_2 - x_3, \ldots, x_{n-1} - x_n\rangle$ is a Jost point, then

$$(x_i - x_j) \cdot \widetilde{(x_i - x_j)} < 0$$

for each i and j. By Property 7, it follows that

$$\mathscr{W}_n(x_1, \ldots, x_n) = \mathscr{W}_n(x_n, \ldots, x_1)$$

or

$$W_n(\xi_1, \ldots, \xi_{n-1}) = W_n(-\xi_{n-1}, \ldots, -\xi_1) \tag{IX.38}$$

when $\langle \xi_1, \ldots, \xi_{n-1} \rangle$ is a Jost point. Since $-I \in \mathscr{L}_+(\mathbb{C})$, (IX.37) and (IX.38) together imply that

$$W_n(\xi_1, \ldots, \xi_{n-1}) = W_n(\xi_{n-1}, \ldots, \xi_1) \tag{IX.39}$$

Since W_n is analytic in $\mathscr{T}^e_{n-1}$ and (IX.39) holds on an open subset of a $\mathbb{R}^{4n-4}$-dimensional subspace, (IX.39) holds throughout $\mathscr{T}^e_{n-1}$, i.e.

$$W_n(z_1, \ldots, z_{n-1}) = W_n(z_{n-1}, \ldots, z_1) \tag{IX.40}$$

for $z = \langle z_1, \ldots, z_{n-1} \rangle \in \mathscr{T}^e_{n-1}$. If $z_j = \xi_j - i\eta_j$ with $\eta_j \in V_+$, then by Theorem IX.16, $W_n(z_1, \ldots, z_{n-1})$ converges to $W_n(\xi_1, \ldots, \xi_{n-1})$ and $W_n(z_{n-1}, \ldots, z_1)$ converges to $W_n(\xi_{n-1}, \ldots, \xi_1)$ in the sense of distributions as $\eta \downarrow 0$. Thus (IX.39) holds for all $\langle \xi_1, \ldots, \xi_{n-1} \rangle \in \mathbb{R}^{4n-4}$ and it follows that

$$\mathscr{W}_n(x_1, \ldots, x_n) = \mathscr{W}_n(-x_n, \ldots, -x_1) \tag{IX.41}$$

for all $\langle x_1, \ldots, x_n \rangle \in \mathbb{R}^{4n}$. Now, define an operator Θ by

$$\Theta\varphi(f_1) \cdots \varphi(f_{n+1})\psi_0 = \varphi(\tilde{\bar{f}}_1) \cdots \varphi(\tilde{\bar{f}}_{n+1})\psi_0$$

and extend Θ to D_0 by real linearity. By (IX.41), Θ is norm-preserving and thus well defined. It is easily checked that $\Theta(\psi_1 + \psi_2) = \Theta(\psi_1) + \Theta(\psi_2)$ and $\Theta(c\psi) = \bar{c}\Theta\psi$; such an operator is called **antilinear**. By Property 8, D_0 is dense in $\mathscr{H}$. So, since $\Theta^2 = I$, Θ extends uniquely to an antiunitary operator on $\mathscr{H}$ which satisfies

$$\Theta\varphi(f)\Theta^{-1} = \varphi(\tilde{\bar{f}}) \qquad \text{for all } f \in \mathscr{S}(\mathbb{R}^4)$$

The existence of such a Θ is just the celebrated **PCT theorem** for the case of a Hermitian scalar field theory.

We remark that some care is needed in using these analyticity arguments. For example, (IX.38) and the analyticity imply that

$$W_n(z_1, \ldots, z_{n-1}) = W_n(-z_{n-1}, \ldots, -z_1) \tag{IX.42}$$

throughout the extended forward tube. But, we *cannot* conclude from this that

$$W_n(\xi_1, \ldots, \xi_{n-1}) = W_n(-\xi_{n-1}, \ldots, -\xi_1) \tag{IX.43}$$

for $\langle \xi_1, \ldots, \xi_{n-1} \rangle \in \mathbb{R}^{4n-4}$ by taking boundary values. $W_n(\xi_1, \ldots, \xi_{n-1})$ is the boundary value of $W_n(z_1, \ldots, z_{n-1})$ as $z_j \to x_j$ in the forward tube. But, if $\eta_j \in V_+$ then $-\eta_j \notin V_+$ so $\langle -z_{n-1}, \ldots, -z_1 \rangle$ is not in the forward tube. Thus the limit of $W_n(-z_{n-1}, \ldots, -z_1)$ in the sense of $\mathscr{S}'(\mathbb{R}^{4n-4})$ may have nothing to do with $W_n(-\xi_{n-1}, \ldots, -\xi_1)$.

The Wightman axioms place fairly strong restrictions on the distributions W_n. As a final illustration of this fact we will use Fourier transform methods to derive the Källen–Lehmann representation of the two-point function W_2. In order to do this we need a theorem about Lorentz invariant measures. For each $m \geq 0$, let $H_m = \{x \in \mathbb{R}^4 \,|\, x \cdot \tilde{x} = m^2,\ x_0 > 0\}$. The sets H_m, which are called **mass hyperboloids**, are invariant under $L_+^\uparrow$. Let j_m be the homeomorphism of H_m onto $\mathbb{R}^3$ (or in the case $m = 0$ onto $\mathbb{R}^3 \backslash 0$) given by $j_m : \langle x_0, x_1, x_2, x_3 \rangle \mapsto \langle x_1, x_2, x_3 \rangle = \mathbf{x}$. Define a measure Ω_m on H_m by setting

$$\Omega_m(E) = \int_{j_m(E)} \frac{d^3x}{\sqrt{m^2 + |\mathbf{x}|^2}}$$

for any measurable set $E \subset H_m$. The measure Ω_m can easily be seen to be $L_+^\uparrow$-invariant. In fact, up to a constant multiple, Ω_m is the only $L_+^\uparrow$-invariant measure on H_m (see the Appendix). Furthermore, every polynomially bounded $L_+^\uparrow$-invariant measure on $\bar{V}_+$ is the sum of a multiple of δ and an integral of the measures Ω_m. We state this fact as a theorem.

Theorem IX.33 Let μ be a polynomially bounded measure with support in $\bar{V}_+$. If μ is $L_+^\uparrow$-invariant, there exists a polynomially bounded measure ρ on $[0, \infty)$ and a constant c so that

$$\int_{\mathbb{R}^4} f \, d\mu = cf(0) + \int_0^\infty \left(\int_{H_m} f \, d\Omega_m \right) d\rho(m)$$

for all $f \in \mathscr{S}(\mathbb{R}^4)$.

Proof See the Appendix to this section.

Theorem IX.34 (Källen–Lehmann representation) Let W_2 be the two-point function of a field theory satisfying the Wightman axioms and the additional condition that $(\psi_0, \varphi(f)\psi_0) = 0$ for all $f \in \mathscr{S}(\mathbb{R}^4)$. Then there exists a polynomially bounded positive measure on $[0, \infty)$ so that for all $f \in \mathscr{S}(\mathbb{R}^4)$,

$$W_2(f) = \int_0^\infty \left(\int_{H_m} \hat{f} \, d\Omega_m \right) d\rho(m)$$

Symbolically,

$$W_2(x) = \int_0^\infty \frac{1}{i} \Delta_+(x; m^2) \, d\rho(m)$$

where

$$\Delta_+(x; m^2) = \frac{i}{2(2\pi)^3} \int_{\mathbb{R}^3} \frac{\exp(-ix_0\sqrt{m^2 + \mathbf{k}^2} + i\mathbf{x}\cdot\mathbf{k})}{\sqrt{m^2 + \mathbf{k}^2}}\, d^3\mathbf{k}$$

Proof Let $f \in \mathscr{S}(\mathbb{R}^4)$. Then

$$\begin{aligned}\iint \overline{f(x)} f(y) W_2(x - y)\, dx\, dy &= (\psi_0, \varphi(\bar{f})\varphi(f)\psi_0) \\ &= \|\varphi(f)\psi_0\|^2 \geq 0\end{aligned}$$

Thus W_2 is a distribution of positive type. By the Bochner–Schwartz theorem, $\check{W}_2$ is a polynomially bounded measure and by Theorem IX.27 the support of $\check{W}_2$ is contained in $\bar{V}_+$. Since $\mathscr{W}_2$ is $\mathscr{L}_+^\uparrow$-invariant, W_2 is invariant and the reader can easily check that this implies that $\check{W}_2$ is $\mathscr{L}_+^\uparrow$-invariant. Thus $\check{W}_2$ satisfies all the hypotheses of Theorem IX.33, so

$$W_2(f) = c\hat{f}(0) + \int_0^\infty \left(\int_{H_m} \hat{f}\, d\Omega_m \right) d\rho(m)$$

for some polynomially bounded measure ρ on $[0, \infty)$ and some constant c.

To conclude the proof we will use the hypothesis that $(\psi_0, \varphi(f)\psi_0) = 0$ for all $f \in \mathscr{S}(\mathbb{R}^4)$ to prove that $c = 0$. Let $g \in \mathscr{S}(\mathbb{R}^4)$ and define $G(a) = (\varphi(g)\psi_0, U(-a, I)\varphi(g)\psi_0)$. Then,

$$\begin{aligned}G(a) &= (\psi_0, \varphi(\bar{g})\varphi(g_{-a}(x))\psi_0) = (W_2 * g_{-a})(\bar{g}) \\ &= (W_2 * g)(\bar{g}_a) = (W_2 * g * \tilde{\bar{g}})(a)\end{aligned}$$

Therefore, $\check{G}$ is the measure $|\check{g}(k)|^2 \check{W}_2$. But

$$G(a) = \int e^{-ia\cdot\lambda}\, d(\varphi(g)\psi_0, E_\lambda \varphi(g)\psi_0)$$

$$= \int e^{-ia\cdot\lambda}\, d(\varphi(g)\psi_0, E_\lambda \varphi(g)\psi_0)$$

so $\check{G}$ is also the measure $(2\pi)^2\, d(\varphi(g)\psi_0, E_\lambda \varphi(g)\psi_0)$. Since the vacuum is unique (Property 3), the mass of $d(\varphi(g)\psi_0, E_\lambda \varphi(g)\psi_0)$ at the origin is $|(\psi_0, \varphi(g)\psi_0)|^2$ which equals zero by hypothesis. Thus $|\check{g}(k)|^2 \check{W}_2$ has no mass at the origin. Since this is true for all $g \in \mathscr{S}(\mathbb{R}^4)$, we conclude that $c = 0$. ∎

We remark that Theorem IX.32 can be combined with microscopic causality to prove analyticity properties for certain distributions arising from commutators of the field. For example, if we define

$$C_2(y - x) = (\psi_0, \varphi(x)\varphi(y)\psi_0) - (\psi_0, \varphi(y)\varphi(x)\psi_0)$$

then by Property 7, C_2 has support in $\bar{V}_+ \cup (-\bar{V}_+)$. Such a distribution can be written $C_2 = R_2 + A_2$ where supp $R_2 \subset \bar{V}_+$ and supp $A_2 \subset -\bar{V}_+$; see Problem 56. R_2 is obviously determined up to a distribution with support at the origin. Since supp $R_2 \subset \bar{V}_+$, the Fourier transform of R_2 is analytic in the tube $\mathbb{R}^4 - iV_+$. For R_2 this can be seen directly from the Källen–Lehmann representation. For a general model, one would like to prove that the higher order commutators C_n can be written as a sum of distributions with supports in cones. The corresponding retarded functions R_n would then have Fourier transforms which are the boundary values of analytic functions. The analyticity properties of the $\hat{R}_n$ are related to the analyticity of the scattering amptitude.

Appendix to IX.8 Lorentz invariant measures

The purpose of this appendix is to prove the facts about Lorentz invariant measures used in Section IX.8. In particular we will prove Theorem IX.33. First we need some general results about measures on product spaces.

Theorem IX.35 (a) Let X be a locally compact space and let $\{T_\alpha\}_{\alpha \in A}$ be a family of homeomorphisms of X into itself. Suppose that there is precisely one (up to constant multiples) Baire measure μ invariant under all the T_α. Let Y be another locally compact space and define $T_\alpha \times I$ by $T_\alpha \times I: \langle x, y\rangle \mapsto \langle T_\alpha x, y\rangle$ for all $\langle x, y\rangle \in X \times Y$. Then any Baire measure ρ on $X \times Y$ invariant under all the maps $T_\alpha \times I$ is of the form $\rho = \mu \otimes \nu$ for some Baire measure ν on Y.

(b) If X and Y are locally compact spaces and $\mu_1 \otimes \nu_1 = \mu_2 \otimes \nu_2$ for nonzero measures $\mu_1, \mu_2, \nu_1, \nu_2$, then $d\mu_1 = c\, d\mu_2$ and $d\nu_1 = c^{-1}\, d\nu_2$.

Proof Let ρ be invariant under the $T_\alpha \times I$ and choose $f \in \kappa(Y)$, the continuous functions of compact support, with $f \geq 0$. Let ρ_f be the map from $\kappa(X)$ to $\mathbb{R}$ defined by $\rho_f: g \mapsto \rho(g \otimes f)$. Since ρ_f is a positive linear form on $\kappa(X)$, it is a Baire measure. In addition ρ_f is invariant under the maps T_α since ρ is invariant under the maps $T_\alpha \times I$, so by hypothesis $\rho_f = c_f \mu$ for some constant c_f. Since, by hypothesis $\mu \neq 0$, we can find a positive function $g \in \kappa(X)$ so that $\mu(g) > 0$. Then $c_f = \rho(g \otimes f)/\mu(g)$ is a positive linear form on $\kappa(Y)$ so $c_f = \nu(f)$ for some Baire measure ν, i.e. $\rho = \mu \otimes \nu$. This proves (a).

To prove (b) we first observe that μ_1 and μ_2 and also ν_1 and ν_2 must have the same sets of zero measure. Let f and g be the characteristic functions of sets E and F in X and Y respectively where $\mu_1(f) \neq 0 \neq \nu_2(g)$. Then $\mu_2(E)/\mu_1(E) = \nu_1(F)/\nu_2(F)$ from which (b) immediately follows. ∎

We will need some information about measures on $\mathbb{R}^n$ and $\mathbb{R}^+$.

Theorem IX.36

(a) Constant multiples of Lebesgue measure are the only translation-invariant Baire measures on $\mathbb{R}^n$.

(b) The only Baire measures on $\mathbb{R}^+ = (0, \infty)$ that are invariant under all the transformations T_a: $x \mapsto e^a x$ (all $a \in \mathbb{R}$) are constant multiples of the measure dx/x.

Proof We begin by proving (a) for the case $n = 1$. We need only show that if μ is translation invariant and $\mu([0, 1]) = 1$, then μ is Lebesgue measure. Since $\mu(\{x\})$ is independent of x and $[0, 1]$ contains infinitely many points, we must have $\mu(\{x\}) = 0$. Thus $\mu([0, 1)) = 1$. Since $[0, 1)$ is a union of n translates of $[0, 1/n)$, we have $\mu([0, 1/n)) = 1/n$ and it easily follows from this that $\mu([0, r)) = r$ for any positive rational number r. Translation invariance then implies that if a and b are rationals and $a < b$, then $\mu((a, b)) = b - a$. But since μ is a Baire measure, it is regular which implies $\mu((a, b)) = b - a$ for all $a < b$. Since μ is determined by its values on finite open intervals, μ must be Lebesgue measure.

We now complete the proof of (a) by induction. Suppose that the only translation invariant measures in $\mathbb{R}^k$ are multiples of $d^k x$ and let ρ be a translation invariant measure on $\mathbb{R}^{k+1} = \mathbb{R}^k \times \mathbb{R}$. Since ρ is invariant under the subgroup of translations of the form $T \times I$ it is of the form $d^k x \otimes d\nu$ by Theorem IX.35a. Since ρ is also invariant under the subgroup of the form $I \times T$ it is of the form $d\mu \otimes dx$. Thus, by Theorem IX.35b, $\rho = c\, d^k x \otimes dx = c\, d^{k+1} x$.

(b) follows from (a) since $\ln: x \to \ln(x)$ is a homeomorphism of $\mathbb{R}^+$ onto $\mathbb{R}$ under which T_a goes over into translation by a. ∎

We are now ready to examine Lorentz invariant measures on $\overline{V}_+$; i.e. polynomially bounded measures with support in $\overline{V}_+$ which are invariant under $\mathscr{L}_+^\uparrow$. $\overline{V}_+$ can be written $\overline{V}_+ = \{0\} \cup (\bigcup_{m=0}^{\infty} H_m)$. Further, the set $\{0\}$ and each of the H_m are taken into themselves by $\mathscr{L}_+^\uparrow$. First we will examine H_m and show that it has only one invariant measure Ω_m (defined in Section 8). Then we will prove Theorem IX.33 which says that any Lorentz

invariant measure on $\bar{V}_+$ can be obtained by "adding up" a delta function at $\langle 0, 0, 0, 0\rangle$ and these invariant measures on the H_m. Although there will be many changes of variable in the following proofs, the idea of all of them is the same: to homeomorphically map the space one is interested in onto a product space $X \times Y$, to analyze the invariant measures on X and Y by Theorem IX.36, and then to determine the invariant measures on $X \times Y$ (and thus on the original space) by using Theorem IX.35.

Lemma The measure $\Omega_m(\cdot)$ on H_m is invariant under $\mathscr{L}_+^\uparrow$.

Proof One straightforward way of seeing that Ω_m is Lorentz invariant is to compute the action of any $\Lambda \in \mathscr{L}_+^\uparrow$ on H_m, proving that the Jacobians work out to keep Ω_m invariant. A more instructive proof first notes that d^4x is $\mathscr{L}_+^\uparrow$-invariant since $\Lambda \in \mathscr{L}_+^\uparrow$ implies $\det \Lambda = 1$. Let $f \in C_0^\infty(0, \infty)$; then since V_+ is $\mathscr{L}_+^\uparrow$-invariant, the measure $f(x \cdot \tilde{x})\chi\, d^4x$ is $\mathscr{L}_+^\uparrow$-invariant where χ is the characteristic function of V_+. Now map V_+ homeomorphically onto $\mathbb{R}^3 \times \mathbb{R}^+$ by h: $\langle x_0, \mathbf{x}\rangle \mapsto \langle \mathbf{x}, y\rangle$ where $y = x \cdot \tilde{x}$. Then $\partial y/\partial x_0 = 2x_0$ so

$$d^4x = \frac{d^3\mathbf{x}\, dy}{2\sqrt{m^2 + x^2}}$$

Thus, the measure

$$\Omega^f(E) = \int_{h[E]} \frac{f(y)\, d^3\mathbf{x}\, dy}{\sqrt{m^2 + \mathbf{x}^2}}$$

is $\mathscr{L}_+^\uparrow$-invariant. If $f_n(y)$ is a sequence in $C_0^\infty(0, \infty)$ converging to $\delta(y - m^2)$, $m > 0$, then Ω^{f_n} converges to Ω_m in $\mathscr{S}'(\mathbb{R}^4)$ and thus Ω_m is $\mathscr{L}_+^\uparrow$-invariant in the sense that $\Omega_m(g(x)) = \Omega_m(g(\Lambda x))$ for all $g \in \mathscr{S}(\mathbb{R}^4)$, $\Lambda \in \mathscr{L}_+^\uparrow$. By a simple argument, this implies $\Omega_m(E) = \Omega_m(\Lambda E)$ for $m > 0$. Since $\Omega_m \to \Omega_0$ in $\mathscr{S}'(\mathbb{R}^4)$ as $m \downarrow 0$ we have also proven the case where $m = 0$. ∎

Because of the way $d\Omega_m$ was constructed in the above proof, some physics literature denotes $d\Omega_m$ by $\delta(x^2 - m^2)\, d^4x$ or even as $\delta(x^2 - m^2)$.

Theorem IX.37 Ω_m is the unique $\mathscr{L}_+^\uparrow$-invariant measure on H_m, $m \geq 0$.

Proof We begin by choosing a new coordinate system for $\mathbb{R}^4$ by letting $\tau = 2^{-1/2}(x_0 - x_3)$, $z = 2^{-1/2}(x_0 + x_3)$, and $\mathbf{x} = \langle x_1, x_2\rangle \in \mathbb{R}^2$. In this new coordinate system the Lorentz inner product is

$$x \cdot \tilde{x} = 2z\tau - \mathbf{x} \cdot \mathbf{x}$$

On any H_m, $m > 0$, we can use τ and $\mathbf{x}$ as coordinates since $z = (2\tau)^{-1}(\mathbf{x} \cdot \mathbf{x} + m^2)$. Notice that if $x \in H_m$ and $m > 0$, then both z and τ are in $(0, \infty)$.

Let ρ be an invariant measure on H_m, $m > 0$, and let s be the homeomorphism of H_m onto $\mathbb{R}^2 \times \mathbb{R}^+$ given by $x \mapsto \langle \mathbf{x}, \tau \rangle$. Let L_a, $a \in \mathbb{R}$, be the linear transformation on $\mathbb{R}^4$ given by $\tau \to e^a\tau$, $z \to e^{-a}z$, $\mathbf{x} \to \mathbf{x}$. Since L_a preserves the form $2z\tau - \mathbf{x} \cdot \mathbf{x}$, $\det L_a = 1$ and L_a: $V_+ \to V_+$, it is a Lorentz transformation and sL_as^{-1}: $\langle \mathbf{x}, \tau \rangle \mapsto \langle \mathbf{x}, e^a\tau \rangle$. Since $s(d\rho)$ is a measure on $\mathbb{R}^2 \times \mathbb{R}^+$ invariant under sL_as^{-1} for all $a \in \mathbb{R}$, we conclude from Theorem IX.36b and Theorem IX.35a that $s(d\rho) = d\mu(\mathbf{x}) \otimes d\tau/\tau$.

Now, let $T_{\mathbf{b}}$: $\mathbb{R}^4 \to \mathbb{R}^4$, $\mathbf{b} \in \mathbb{R}^2$ be the transformation

$$T_{\mathbf{b}}\colon \langle \tau, z, \mathbf{x} \rangle \mapsto \langle \tau, z + \mathbf{b} \cdot \mathbf{x} + \tfrac{1}{2}|\mathbf{b}|^2\tau, \mathbf{x} + \tau\mathbf{b} \rangle$$

A short calculation shows that $T_{\mathbf{b}} \in L_+^\uparrow$. It is clear that $sT_{\mathbf{b}}s^{-1}$: $\langle \mathbf{x}, \tau \rangle \mapsto \langle \mathbf{x} + \tau\mathbf{b}, \tau \rangle$. Let t: $\langle \mathbf{x}, \tau \rangle \mapsto \langle \mathbf{x}/\tau, \tau \rangle$. Then t: $\mathbb{R}^2 \times \mathbb{R}^+ \mapsto \mathbb{R}^2 \times \mathbb{R}^+$ and $tsT_{\mathbf{b}}s^{-1}t^{-1}$: $\langle \mathbf{x}, \tau \rangle \mapsto \langle \mathbf{x} + \mathbf{b}, \tau \rangle$. Using Theorems IX.36a and IX.35a we conclude that $ts(d\rho) = d^2x \otimes dv(\tau)$; i.e. $s(d\rho) = d^2x \otimes dv(\tau)/\tau^2$.

Since $s(d\rho) = d\mu \otimes d\tau/\tau$ and $s(d\rho) = d^2x \otimes dv(\tau)/\tau^2$, we conclude by Theorem IX.35b that $s(d\rho) = c\, d^2x \otimes d\tau/\tau$. Since s sets up a one-to-one correspondence between the measures on H_m and the measures on $\mathbb{R}^2 \times \mathbb{R}^+$, it follows that there is at most one (up to constant multiples) measure on H_m invariant under $\mathscr{L}_+^\uparrow$. By the lemma we know there is at least one such measure, so there is exactly one.

The proof for the case $m = 0$ is similar. We only note first that the set $\{x \mid \tau = 0\}$ must have ρ-measure zero. ∎

Proof of Theorem IX.33 Let μ be a polynomially bounded measure invariant under $\mathscr{L}_+^\uparrow$, with support in $\overline{V}_+$. Let χ_0 be the characteristic function of H_0, χ the characteristic function of $\bigcup_{m>0} H_m$. Then $\chi_0\mu$ is $\mathscr{L}_+^\uparrow$-invariant, so $\chi_0\mu = e\Omega_0$, i.e. $\mu = \mu(\{0\})\delta_0 + e\Omega_0 + \chi\mu$. Let j be the homeomorphism of $\bigcup_{m>0} H_m$ defined by j: $\langle x_0, \mathbf{x} \rangle \mapsto \langle \mathbf{x}/x \cdot \tilde{x}, x \cdot \tilde{x} \rangle$. For each $\Lambda \in L_+^\uparrow$, $j\Lambda j^{-1}$ acts on $\mathbb{R}^3 \times \mathbb{R}^+$ by a product action $\Lambda_s \times I$. The measure $j(\chi\mu)$ is invariant under the maps $\Lambda_s \times I$. By Theorem IX.37 there is a unique measure Ω on $\mathbb{R}^3$ invariant under all Λ_s and $\Omega = c_m j(\Omega_m)$ for each m. By Theorem IX.35a, $h(\chi\mu) = \Omega \otimes \tilde{\rho}$ for some Baire measure $\tilde{\rho}$ on $(0, \infty)$. That is, for $f \in \mathscr{S}(\mathbb{R}^4)$

$$\int_{\overline{V}_+} f(x)\, d\mu(x) = \int_{\mathbb{R}^+} \left(\int_{\mathbb{R}^3} f(j^{-1}(x))\, d\Omega \right) d\tilde{\rho}(m)$$

$$= \int_{\mathbb{R}^+} \left(\int_{H_m} f(x) c_m\, d\Omega_m \right) d\tilde{\rho}(m)$$

Now define ρ on $[0, \infty)$ by $\rho = c_m \tilde{\rho} + e\delta_0$. Then,

$$\int_{\mathbb{R}^n} f(x)\, d\mu(x) = \mu(\{0\}) f(0) + \int_{m \geq 0} \left(\int f(x)\, d\Omega_m \right) d\rho(m)$$

The fact that ρ is polynomially bounded follows from the polynomial boundedness of μ. ∎

IX.9 Restriction to submanifolds

Let M be a hyperplane or a compact submanifold of $\mathbb{R}^n$ of dimension $n-1$ or less. In this section we consider the problem of which $f \in L^2(\mathbb{R}^n)$ can be restricted in a natural way to M. Since M has Lebesgue measure zero in $\mathbb{R}^n$, we will not be able to restrict every f to M. We only expect to be able to restrict those f such that there is a distinguished element in the equivalence class of f which is suitably smooth. For example, an $f \in \mathcal{S}(\mathbb{R}^n)$ has a natural restriction $T_M f$ given by merely taking the values of f on M. The idea of our approach is to find a Banach space B with $\mathcal{S}(\mathbb{R}^n) \subset B \subset L^2(\mathbb{R}^n)$ so that for $f \in \mathcal{S}(\mathbb{R}^n)$, $\|T_M f\|_{L^2(M)} \leq C \|f\|_B$. If $\mathcal{S}(\mathbb{R}^n)$ is dense in B, then we can use the B.L.T. theorem to extend T_M to all of B. A second approach to the restriction problem is discussed in the Notes to Section IX.10.

What shall we take for the Banach space B? Our experience suggests that smoothness conditions on f are equivalent to decay bounds of $\hat{f}$ so it is natural to try to use the Sobolev spaces W_m. For notational convenience we introduce the **weighted L^2 space** L^2_m. We say $f \in L^2_m(\mathbb{R}^n)$ if and only if $\hat{f} \in W_m$, i.e., if and only if

$$\int_{\mathbb{R}^n} (1 + |x|^2)^m |f(x)|^2\, dx < \infty$$

There is a natural question which is dual to the restriction problem that we have posed. Namely, given $f \in L^2(M)$, we can associate f with a tempered distribution $T_M^* f$ on $\mathbb{R}^n$ with the action $T_M^* f$: $\varphi \to \int_M f(x)\varphi(x)\, d\omega$ where ω is the natural measure (see below) on M. What are the growth properties of $\mathcal{F}_M f \equiv \widehat{T_M^* f}$? We begin by solving these two problems for hyperplanes.

Theorem IX.38 Let $f \in \mathcal{S}(\mathbb{R}^n)$ and suppose that M is a plane in $\mathbb{R}^n$ of codimension k, $1 \leq k \leq n-1$.

(a) Let $T_M f$ be the restriction of f to M. Then there is a constant C (independent of f) so that $\|T_M f\|_{L^2(M)} \leq C\|f\|_{W_m}$ for all $m > k - \frac{1}{2}$. Thus T_M extends uniquely to a bounded map of W_m into $L^2(M)$.

(b) Let $d_M x$ be Lebesgue measure on M (defined for example by translating M to the origin and choosing an orthonormal basis) and let $f \in L^2(M, d_M x)$. Define

$$(\mathscr{F}_M f)(\lambda_1, \ldots, \lambda_n) = \frac{1}{(2\pi)^{n/2}} \int_M e^{-ix\cdot\lambda} f(x)\, d_M x \qquad \text{(IX.44)}$$

Then $\mathscr{F}_M f$ is the Fourier transform of f regarded as a tempered distribution and $\mathscr{F}_M f \in L^2_m(\mathbb{R}^n)$ for all $m < -k + \frac{1}{2}$.

Proof We will give a proof for the case $n = 2$, $k = 1$. The proof of the general case uses the same ideas and is left as an exercise (Problem 57). Since both the hypotheses and conclusions are invariant under translations and rotations of M, we may assume that $M = \{\langle x_1, 0\rangle \mid x_1 \in \mathbb{R}\}$.

To prove (a), let $m > \frac{1}{2}$. Then

$$|f(x_1, 0)| \leq \int \left| \int \frac{e^{ix_1\lambda_1}}{2\pi} \hat{f}(\lambda_1, \lambda_2)\, d\lambda_1 \right| d\lambda_2$$

$$\leq \left(\int \frac{d\lambda_2}{(1 + \lambda_2^2)^m} \right)^{1/2} \left(\int (1 + |\lambda_2|^2)^m \left| \int e^{ix_1\lambda_1} \hat{f}(\lambda_1, \lambda_2) \frac{d\lambda_1}{2\pi} \right|^2 d\lambda_2 \right)^{1/2}$$

so, by the Plancherel theorem in one variable,

$$\int |f(x_1, 0)|^2\, dx_1 \leq C \int \left(\int (1 + |\lambda_2|^2)^m \left| \int e^{ix_1\lambda_1} \hat{f}(\lambda_1, \lambda_2) \frac{d\lambda_1}{\sqrt{2\pi}} \right|^2 d\lambda_2 \right) dx_1$$

$$= C \int (1 + |\lambda_2|^2)^m |\hat{f}(\lambda_1, \lambda_2)|^2\, d\lambda_1\, d\lambda_2$$

$$\leq C \int (1 + |\lambda_1|^2 + |\lambda_2|^2)^m |\hat{f}(\lambda_1, \lambda_2)|^2\, d\lambda_1\, d\lambda_2$$

$$= C\|f\|_{W_m}$$

Thus, the restriction map $T_M f = f(\cdot, 0)$ extends to a bounded map of W_m into $L^2(M)$.

Now, suppose that $g \in L^2(M, d_M x) = L^2(\mathbb{R})$. Let χ_n be the characteristic function of $(-n, n)$. Then $\chi_n(x_1) g(x_1) \delta(x_2)$ is a distribution on $\mathbb{R}^2$ with compact support, so by Theorem IX.5,

$$\widehat{\chi_n g\delta}(\lambda_1, \lambda_2) = \frac{1}{2\pi} \int e^{-i\lambda_1 x_1} \chi_n(x_1) g(x_1)\, dx_1$$

If $\varphi \in \mathscr{S}(\mathbb{R}^2)$, then

$$\iint \left(\frac{1}{2\pi}\int e^{-i\lambda_1 x_1}\chi_n(x_1)g(x_1)\,dx_1\right)\varphi(\lambda_1,\lambda_2)\,d\lambda_1\,d\lambda_2$$

$$\longrightarrow \iint \left(\frac{1}{2\pi}\int e^{-i\lambda_1 x_1}g(x_1)\,dx_1\right)\varphi(\lambda_1,\lambda_2)\,d\lambda_1\,d\lambda_2$$

so, since $\chi_n g \to g$ weakly and the Fourier transform is weakly continuous, $(2\pi)^{-1}\int e^{-i\lambda_1 x_1}g(x_1)\,dx_1$ is just the Fourier transform of $g(x_1)\delta(x_2)$ as a distribution on $\mathbb{R}^2$. To complete the proof, we let $m < -\frac{1}{2}$. Then

$$\iint (1 + |\lambda_1|^2 + |\lambda_2|^2)^m |(\mathscr{F}_{\mathbb{R}} g)(\lambda_1,\lambda_2)|^2\,d\lambda_1\,d\lambda_2$$

$$\leq (2\pi)^{-1}\iint (1 + |\lambda_2|^2)^m |\hat{g}(\lambda_1)|^2\,d\lambda_1\,d\lambda_2$$

$$\leq (2\pi)^{-1}\left(\int (1 + |\lambda_2|^2)^m\,d\lambda_2\right)\|g\|^2_{L^2(\mathbb{R})}$$

so $\mathscr{F}_{\mathbb{R}} g \in L^2_m(\mathbb{R}^2)$. ∎

We turn now to the case where M is a compact submanifold.

Definition A **hypersurface** M in $\mathbb{R}^n$ is a set of points with the following property: there is a real-valued C^∞ function F on $\mathbb{R}^n$ so that $M = \{x \mid F(x) = 0\}$ and so that $\nabla F = \langle \partial F/\partial x_1, \ldots, \partial F/\partial x_n\rangle \neq 0$ at each $x \in M$. More generally, a **regularly imbedded submanifold of codimension k** is the set of points where k real-valued C^∞ functions vanish with the additional property that the Jacobian matrix $\{\partial F_i/\partial x_j\}_{1\leq i\leq k,\ 1\leq j\leq n}$ have rank k at each point in M.

For simplicity of notation we will discuss only the case of codimension one. Once F is given, the hypersurface (and more generally, regularly imbedded submanifolds) carries a natural measure. We will describe it in a neighborhood of $x \in M$. Since $\nabla F(x) \neq 0$, $\partial F/\partial x_\ell \neq 0$ for some ℓ. By the implicit function theorem of advanced calculus we can find a neighborhood N of x and a smooth function h_ℓ on $\mathbb{R}^{n-1}$ so that $x_\ell = h_\ell(x_1, \ldots, \hat{x}_\ell, \ldots, x_n)$ for all $\langle x_1, \ldots, x_n\rangle \in N \cap M$, where $\langle x_1, \ldots, \hat{x}_\ell, \ldots, x_n\rangle$ means omit the ℓth coordinate. For each $S \subset (N \cap M)$, we define

$$\omega_N(S) = \int_{h_\ell^{-1}(S)} \frac{dx_1 \cdots d\hat{x}_\ell \cdots dx_n}{|\partial F/\partial x_\ell|}$$

Then by the chain rule and the Jacobian formula for change of variables the measure ω_N is independent of which ℓ with $\partial F/\partial x_\ell \neq 0$ we chose. By piecing the measures ω_N together we can get a natural measure on all of M. The reader can check that the natural measure on S^{n-1} (the surface of the unit ball in $\mathbb{R}^n$) is just the usual spherical measure if

$$F(x_1, \ldots, x_n) = \frac{1}{2}\left(\sum_{i=1}^{n} x_i^2 - 1\right)$$

We remark that the measure we have constructed above is F dependent. But, if M is compact, then any two such measures are absolutely continuous with respect to one another and their Radon–Nikodym derivatives are bounded from above and below by positive constants. Thus the corresponding L^2-spaces on M are the same in the sense that their norms are equivalent. We warn the reader that there is a natural measure on M which can be constructed geometrically but which may differ from the ones we have constructed; see the Notes. If M is compact, then the L^2 space of this geometric measure is the same as the L^2 spaces of the F-dependent measures.

Theorem IX.39 Let M be a regularly imbedded compact submanifold in $\mathbb{R}^n$ of codimension k given by k C^∞ functions $F_1, \ldots, F_k$. We denote by ω the natural induced measure on M. Suppose that $f \in \mathscr{S}(\mathbb{R}^n)$.

(a) Let $T_M f$ be the restriction of f to M. Then for all $m > k - \frac{1}{2}$, there is a constant C (independent of f) so that $\|T_M f\|_{L^2(M, d\omega)} \leq C\|f\|_{W_m}$ so T_M extends uniquely to a bounded map of W_m into $L^2(M, d\omega)$.

(b) Let $f \in L^2(M, d\omega)$ and define

$$(\mathscr{F}_M f)(\lambda_1, \ldots, \lambda_n) = \frac{1}{(2\pi)^{n/2}} \int_M e^{-ix\cdot\lambda} f(x)\, d\omega \qquad \text{(IX.45)}$$

Then $\mathscr{F}_M f$ is the Fourier transform of the tempered distribution on $\mathbb{R}^n$ associated to f, $\mathscr{F}_M f$ is in $C^\infty(\mathbb{R}^n)$, and $\mathscr{F}_M f \in L^2_m(\mathbb{R}^n)$ for all $m < -k + \frac{1}{2}$.

Proof As before, we only give the proof in the case of codimension one. The proof consists of essentially the same computations as in Theorem IX.38, except that we must break the manifold up into a finite number of pieces each of which we flatten out so we can use the Plancherel theorem. In this way we will prove (b). We then avoid the computation in (a) by a duality argument.

Let $f \in L^2(M, d\omega)$. Then f can be associated with a distribution of compact support under the action

$$\varphi \mapsto \int_M f(x)\varphi(x)\, d\omega$$

Since this distribution has compact support, Theorem IX.5 implies that the formula (IX.45) gives its Fourier transform. $\mathscr{F}_M f$ is in C^∞ by the Paley–Wiener theorem for distributions.

By using the implicit function theorem and the compactness of M, we can find a decomposition of M into disjoint measurable sets $S_1, \ldots, S_N$:

$$S_j = \{\langle x_1, \ldots, x_n\rangle \mid x_{\ell(j)} = h_j(x_1, \ldots, \hat{x}_{\ell(j)}, \ldots, x_n), \langle x_1, \ldots, \hat{x}_{\ell(j)}, \ldots, x_n\rangle \in V_j\}$$

where V_j is a measurable subset of $\mathbb{R}^{n-1}$, $c_1 < (\partial F/\partial x_{\ell(j)})(y) < c_2$ for all $y \in S_j$, and $c_1 > 0$, $c_2 < \infty$. Define

$$G_j(\lambda) = (2\pi)^{-n/2} \int_{S_j} e^{-i\lambda \cdot x} f(x)\, d\omega$$

For simplicity of notation we assume that $\ell(j) = n$. Then

$$G_j(\lambda) = (2\pi)^{-n/2} \int_{V_j} \exp\Bigl(-i\lambda_n h_j(x_1, \ldots, x_{n-1}) - i\sum_1^{n-1} \lambda_i x_i\Bigr) \times \left(\frac{f(x_1, \ldots, x_{n-1}, h_j(x_1, \ldots, x_{n-1}))}{\dfrac{\partial F}{\partial x_n}(x_1, \ldots, x_{n-1}, h_j(x_1, \ldots, x_{n-1}))}\right) dx_1 \cdots dx_{n-1}$$

so the same computation as in the proof of Theorem IX.38b implies that for $m < -\frac{1}{2}$, we can use the $(1+\lambda^2)^m$ factor to control the λ_n integration and then the Plancherel theorem to conclude

$$\|G_j\|^2_{L^2_m(\mathbb{R}^n)} \leq C \int_{V_j} \frac{|f(x_1, \ldots, x_{n-1}, h_j(x_1, \ldots, x_{n-1})|^2}{\left|\dfrac{\partial F}{\partial x_n}(x_1, \ldots, x_{n-1}, h_j(x_1, \ldots, x_{n-1})\right|^2} dx_1 \cdots dx_{n-1}$$

$$\leq \frac{C}{c_1} \|f\|^2_{L^2(M \cap S_j, d\omega)}$$

Summing from 1 to N we conclude that there is a constant $\tilde{C}$ so that $\|\mathscr{F}_M f\|_{L^2_m(\mathbb{R}^n)} \leq \tilde{C}\|f\|_{L^2(M, d\omega)}$ for all f. This proves (b).

We have just seen that $\mathscr{F}_M$: $L^2(M, d\omega) \to L^2_{-m}(\mathbb{R}^n)$ is bounded if $m > \frac{1}{2}$. We can identify $L^2_m(\mathbb{R}^n)$ with the dual of $L^2_{-m}(\mathbb{R}^n)$ by associating to each $f \in L^2_m(\mathbb{R}^n)$ the functional

$$g \mapsto \int_{\mathbb{R}^n} \overline{f(x)} g(x)\, dx$$

Thus, $\mathscr{F}_M^*$ maps $L_m^2(\mathbb{R}^n)$ boundedly into $L^2(M, d\omega)$. So we can uniquely associate with each $f \in W_m$ a function $T_M f = \mathscr{F}_M^*(\hat{f})$ in $L^2(M, d\omega)$, so that if $f \in \mathscr{S}(\mathbb{R}^n)$, this mapping is just the restriction of f to M. Moreover, $\|T_M f\|_{L^2(M, d\omega)} \leq C\|f\|_{W_m}$. ∎

One is often interested in knowing how the restriction maps change as the submanifold M changes. Consider the case where $M = S^{n-1}$, the $(n-1)$-sphere in $\mathbb{R}^n$, and let $S_\lambda^{n-1} = \{x \in \mathbb{R}^n \mid \sum_{i=1}^n x_i^2 - \lambda = 0\}$. Theorem IX.39 implies that the restriction map T_λ is a bounded map from $W_m(\mathbb{R}^n)$ into $L^2(S_\lambda^{n-1}, d\omega)$ for each λ if $m > \frac{1}{2}$. Define $(U_\lambda f)(x) = f(\lambda x)$; then U_λ: $L^2(S_\lambda^{n-1}, d\omega) \to L^2(S^{n-1}, d\omega)$. We would like to know the continuity properties of the family of maps $U_\lambda T_\lambda$: $W_m(\mathbb{R}^n) \to L^2(S^{n-1}, d\omega)$.

Definition A function g from a metric space $\langle X, \rho\rangle$ to a Banach space $\langle B, \|\cdot\|\rangle$ is called **Hölder continuous of order α**, $\alpha \in (0, 1]$, if for each $x \in X$, there is a $\delta > 0$ such that $\|g(x) - g(y)\| \leq C\rho(x, y)^\alpha$ for all y satisfying $\rho(x, y) < \delta$.

Theorem IX.40 Let $R_\lambda = U_\lambda T_\lambda$ be the family of restriction maps defined above with $m > \frac{1}{2}$. Then for each $f \in W_m(\mathbb{R}^n)$, $R_\lambda f$ is Hölder continuous of order α as an $L^2(S^{n-1}, d\omega)$-valued function of λ for each α with $0 < \alpha < m - \frac{1}{2}$.

Proof We sketch the proof leaving the details to the reader (Problem 58). Let $f \in L^2(S^{n-1}, d\omega)$ and define the dilated Fourier transform by

$$(\mathscr{F}^{(\lambda)} f)(k) = (2\pi)^{-n/2} \int_{S^{n-1}} e^{-ik \cdot \lambda x} f(x)\, d\omega$$

Notice that $|e^{-ik \cdot \lambda x} - e^{-ik \cdot \lambda' x}| \leq C|\lambda - \lambda'|^\alpha |k|^\alpha$ for any $\alpha \leq 1$. Using this, one proves that

$$\|\mathscr{F}^{(\lambda)} f - \mathscr{F}^{(\lambda')} f\|_{L_{-m}^2(\mathbb{R}^n)} \leq C|\lambda - \lambda'|^\alpha \|f\|_{L^2(S^{n-1}, d\omega)}$$

if $\alpha < m - \frac{1}{2}$. Since $R_\lambda f = (\mathscr{F}^{(\lambda)})^* \hat{f}$ (under the duality described in the proof of Theorem IX.39) we conclude from this that

$$\|R_\lambda f - R_{\lambda'} f\| \leq C_\alpha |\lambda - \lambda'|^\alpha \|f\|_{W_m}$$ ∎

We remark that it is possible to prove the following stronger result: Suppose $n + \frac{1}{2} < m \leq n + \frac{3}{2}$; then $R_\lambda f$, regarded as a map of $W_m(\mathbb{R}^n)$ into $L^2(S^{n-1}, d\omega)$ is n times differentiable and the nth derivative is Hölder continuous of order α for all $0 < \alpha < m - n - \frac{1}{2}$.

Our final topic in this section is the investigation of the map

$$f \mapsto \widehat{((k^2 - \lambda)^{-1} \hat{f})}$$

for λ positive. We are interested in this map because it is just the unbounded inverse $(-\Delta - \lambda)^{-1}$ for $\lambda > 0$. We will continue our study of $(-\Delta - \lambda)^{-1}$ in Section XIII.7, where we study the spectral properties of certain quantum-mechanical Hamiltonians. The idea of the following theorem is that $(k^2 - \lambda)^{-1}$ is singular only on $S^n_{\lambda^{1/2}}$, the sphere of radius $\lambda^{1/2}$, so if the restriction of $\hat{f}$ to $S^n_{\lambda^{1/2}}$ is zero we expect that $f \mapsto \widehat{(k^2 - \lambda)^{-1} \hat{f}}$ should not be too singular. For convenience, we denote the norm on $L^2_\alpha(\mathbb{R}^n)$ by $\|\cdot\|_\alpha$.

Theorem IX.41 Let $f \in L^2_\alpha(\mathbb{R}^n)$ for some $\alpha > \frac{1}{2}$ and suppose that the restriction of $\hat{f}$ (given by Theorem IX.39) to the sphere of radius $\lambda^{1/2}$ ($\lambda > 0$) is the zero function. Then for each $\varepsilon > 0$,

$$B_\lambda f \equiv \widehat{(k^2 - \lambda)^{-1} \hat{f}} \in L^2_{\alpha - 1 - 2\varepsilon}$$

Moreover, for each $\varepsilon > 0$, $\alpha > \frac{1}{2}$, and $\lambda > 0$, there is a constant C so that

$$\|B_\lambda f\|_{\alpha - 1 - 2\varepsilon} \leq C \|f\|_\alpha$$

for all $f \in L^2_\alpha(\mathbb{R}^n)$ such that $\hat{f}$ vanishes on $S^n_{\lambda^{1/2}}$. C remains bounded if λ varies through a compact subset of $(0, \infty)$.

We will prove Theorem X.41 by a series of lemmas. The first is a direct consequence of the fact that L^2_α is the set of Fourier transforms of the Sobolev space W_α and the proof of Proposition 2 in Section IX.6.

Lemma 1 Let F be a C^∞ function so that all the derivatives of F are bounded. Then $f \mapsto \widehat{(F\hat{f})}$ is a bounded map on each L^2_α.

Our technique for proving Theorem IX.41 will be to prove the theorem first in the case $n = 1$ and then to use this special case along with a "cutting and pasting" argument to do the general case.

Lemma 2 Let $f \in L^2_\alpha(\mathbb{R})$ with $\alpha > \frac{1}{2}$ (so that $f \in L^1(\mathbb{R})$). Suppose that $\int_{-\infty}^{\infty} f(x)\, dx = 0$. Then,

(a) There is a one-parameter family of tempered distributions satisfying

$k\hat{g}(k) = \hat{f}(k)$. Each is a continuous function and there is a unique one g with $\lim_{x\to\pm\infty} g(x) = 0$.

(b) For each sufficiently small $\varepsilon > 0$, g obeys the bound

$$|g(x)| \leq C\|f\|_\alpha (1 + |x|^2)^{-\frac{1}{2}(\alpha - \frac{1}{2} - \varepsilon)} \tag{IX.46}$$

where C depends only on α and ε.

Proof Let $g(x)$ be defined by

$$g(x) = i\int_{-\infty}^{x} f(y)\,dy = -i\int_{x}^{\infty} f(y)\,dy \tag{IX.47}$$

Suppose that $x < 0$ and choose $\varepsilon > 0$ small enough so that $\alpha > \frac{1}{2} + \varepsilon$. Then

$$|g(x)|^2 \leq \left| \int_{-\infty}^{x} |f(y)|(1 + |y|^2)^{\frac{1}{2}\alpha}(1 + |y|^2)^{-\frac{1}{4}-\frac{1}{2}\varepsilon}(1 + |x|^2)^{-\frac{1}{2}(\alpha-\frac{1}{2}-\varepsilon)}\,dy \right|^2$$

$$\leq (1 + |x|^2)^{-(\alpha-\frac{1}{2}-\varepsilon)}\|f\|_\alpha^2 \int_{-\infty}^{\infty} (1 + |y|^2)^{-\frac{1}{2}-\varepsilon}\,dy$$

For $x \geq 0$, one uses a similar argument using the second equality in (IX.47). Since $f \in L^1(\mathbb{R})$, g is absolutely continuous and $g'(x) = if(x)$, thus $k\hat{g}(k) = \hat{f}(k)$. By the hypothesis on f, $g(x) \to 0$ as $x \to \pm\infty$. If g_β is another tempered distribution satisfying $k\hat{g}_\beta = \hat{f}$, then $k(\hat{g} - \hat{g}_\beta) = 0$, so $\hat{g} - \hat{g}_\beta$ has support at the origin. This implies that $\hat{g}_\beta - \hat{g}$ is a finite linear combination of the delta function and its derivatives. Since $k(\hat{g}_\beta - \hat{g}) = 0$, the coefficients of the derivative terms vanish, so $\hat{g}_\beta = \hat{g} + \beta\hat{\delta}_0$. It follows that $g_\beta = g + \beta(2\pi)^{-1/2}$. This shows that $g_\beta \to 0$ at $\pm\infty$ if and only if $\beta = 0$. ∎

We can now prove the one-dimensional case of Theorem IX.41.

Lemma 3 Let $\lambda > 0$ and $\alpha > \frac{1}{2}$. Suppose that $h \in L^2_\alpha(\mathbb{R})$ and $\hat{h}(\pm\lambda^{1/2}) = 0$. Then, there is a continuous function g going to zero at ∞ so that $(k^2 - \lambda)\hat{g} = \hat{h}$. Moreover, g obeys

$$|g(x)| \leq D_\lambda \|h\|_\alpha (1 + |x|^2)^{-\frac{1}{2}(\alpha-\frac{1}{2}-\varepsilon)} \tag{IX.48}$$

where D_λ is a constant depending only on λ, α, and ε. For fixed α and ε, D_λ is bounded for λ in any compact subset of $(0, \infty)$.

Proof By a simple argument using the formula $\widehat{e^{i\gamma x} f(x)} = \hat{f}(k - \gamma)$, one can see that Lemma 2 implies that if $\hat{h}(\gamma) = 0$, then there is a g obeying (IX.46) so that $(k - \gamma)\hat{g} = \hat{h}$. We will denote such a g by $\widehat{(k-\gamma)^{-1}\hat{h}}$. Choose

a C^∞ function χ so that $\chi(k) = 0$ if $k < -\frac{1}{2}\lambda^{1/2}$ and $\chi(k) = 1$ if $k > \frac{1}{2}\lambda^{1/2}$ and define

$$F_1(k) = (k + \lambda^{1/2})^{-1}\chi(k), \qquad F_2(k) = (k - \lambda^{1/2})^{-1}(1 - \chi(k))$$

so that $(k - \lambda^{1/2})^{-1}F_1 + (k + \lambda^{1/2})^{-1}F_2 = (k^2 - \lambda)^{-1}$. Let $f_i = \widetilde{F_i h}$. By Lemma 1, $\|f_i\|_\alpha \le C_{i,\alpha}\|h\|_\alpha$. Let $\hat{g} = (k - \lambda^{1/2})^{-1}\hat{f}_1 + (k + \lambda^{1/2})^{-1}\hat{f}_2$. Then $(k^2 - \lambda)\hat{g} = \hat{h}$ and

$$\begin{aligned} |g(x)| &\le C[\|f_1\|_\alpha + \|f_2\|_\alpha](1 + |x|^2)^{-\frac{1}{2}(\alpha - \frac{1}{2} - \varepsilon)} \\ &\le D\|h\|_\alpha(1 + |x|^2)^{-\frac{1}{2}(\alpha - \frac{1}{2} - \varepsilon)} \end{aligned}$$

That D_λ is bounded as λ runs through a compact subset of $(0, \infty)$ is a simple consequence of the above proof. ∎

Note that by (IX.48),

$$\int |g(x)|^2(1 + |x|^2)^{\alpha - 1 - 2\varepsilon}\, dx \le D^2\|h\|_\alpha^2 \int (1 + |x|^2)^{-\frac{1}{2} - \varepsilon}\, dx$$

so that Lemma 3 is, indeed, a strengthened version of Theorem IX.41 in the case $n = 1$.

Lemma 4 Let $f \in L^2_\alpha(\mathbb{R}^n)$ with $\alpha > \frac{1}{2}$ and suppose that $\hat{f}$ vanishes on the sphere of radius λ. Then for almost every $p \in \mathbb{R}^{n-1}$,

$$h_p(y) \equiv (2\pi)^{-(n-1)/2} \int e^{-i(p_1x_1 + \cdots + p_{n-1}x_{n-1})} f(x_1, \ldots, x_{n-1}, y)\, d^{n-1}x$$

is in $L^2_\alpha(\mathbb{R})$ and for almost every $p \in \mathbb{R}^{n-1}$ with $|p| \le \lambda$, $\hat{h}_p(\pm\sqrt{\lambda^2 - |p|^2}) = 0$.

Proof If f were in $L^1(\mathbb{R}^n)$, the conclusion of the lemma would be trivial, but we must work a little harder. Since $f(x_1, \ldots, x_{n-1}, y)(1 + \sum_1^{n-1} x_i^2 + y^2)^{\alpha/2}$ is in $L^2(\mathbb{R}^n)$, we know that $f(x_1, \ldots, x_{n-1}, y)(1 + y^2)^{\alpha/2}$ is in $L^2(\mathbb{R}^n)$. Thus, by the Plancherel theorem,

$$\int |h_p(y)|^2(1 + |y|^2)^\alpha\, dy\, d^{n-1}p < \infty$$

It follows that for almost all p, $h_p(\cdot) \in L^2_\alpha(\mathbb{R})$. Now, choose $f_m \in \mathscr{S}(\mathbb{R}^n)$ so that $\|f - f_m\|_\alpha \to 0$. By Theorem IX.39, $\hat{f}_m \to \hat{f}$ in $L^2(S^{n-1}_\lambda)$. Therefore, by passing to a subsequence if necessary, we may assume that:

(1) $\hat{f}_m(p, \pm\sqrt{\lambda - |p|^2}) \to 0$ for almost all $p \in \mathbb{R}^{n-1}$ with $|p|^2 < \lambda$
(2) $\|f_m - f\|_\alpha \le 4^{-m}$.

Define

$$h_p^{(m)}(y) = (2\pi)^{-(n-1)/2} \int \exp\left(-i \sum_{i=1}^{n-1} p_i x_i\right) f_m(x_1, \ldots, x_{n-1}, y)\, d^{n-1}x$$

We claim that $\|h_p^{(m)} - h_p\|_{L_\alpha^2(\mathbb{R})} \to 0$ a.e. in p. For by the argument at the beginning of the proof $\int \|h_p^{(m)} - h_p\|_\alpha^2\, d^{n-1}p \le 4^{-2m}$. Thus, for each m, the set $U_m = \{p \mid \|h_p^{(m)} - h_p\|_\alpha < 2^{-m}\}$ has a complement with measure less than 4^{-m}. Let $T_m = \bigcap_{n \ge m} U_n$ and let μ denote Lebesgue measure. Then $\mu(\mathbb{R}^{n-1} \backslash T_m) \le 4^{-m+1}$ so $\mu(\mathbb{R}^{n-1} \backslash \bigcup_m T_m) = 0$. But on each T_m, $h_p^{(m)} \to h_p$ in $L_\alpha^2(\mathbb{R})$ so $\|h_p^{(m)} - h_p\|_\alpha \to 0$ for almost all p. Therefore, by Theorem IX.39, $\hat{h}_p^{(m)}(\pm\sqrt{\lambda^2 - |p|^2}) \to \hat{h}_p(\pm\sqrt{\lambda^2 - |p|^2}) = \hat{f}(p, \sqrt{\lambda^2 - |p|^2})$ for almost all p with $|p|^2 < \lambda$. Since $\hat{h}_p^{(m)}(\pm\sqrt{\lambda - |p|^2}) = \hat{f}_m(p, \pm\sqrt{\lambda - |p|^2})$, (1) implies that $\hat{h}_p(\pm\sqrt{\lambda - |p|^2}) = 0$. ∎

Lemma 5 Fix $\lambda > 0$ and let

$$V = \left\{k \,\middle|\, \sum_{i=1}^{n-1} |k_i|^2 + |k_n - \lambda^{1/2}|^2 < \tfrac{1}{4}\lambda\right\} \subset \mathbb{R}^n.$$

Let $f \in L_\alpha^2(\mathbb{R}^n)$, $\alpha > \frac{1}{2}$, and suppose that $\hat{f}$ has support in V and that $\hat{f}\,|S_\lambda^{n-1} = 0$. Then

$$B_\lambda f = \widehat{(k^2 - \lambda)^{-1}\hat{f}} \in L_{\alpha-1-2\varepsilon}^2(\mathbb{R}^n) \qquad \text{and} \qquad \|B_\lambda f\|_{\alpha-1-2\varepsilon} \le C'\|f\|_\alpha.$$

Proof Define $h_p(y)$ as in Lemma 4 and notice that by the argument at the start of the proof of Lemma 4 we have

$$\int \|h_p\|_\alpha^2\, d^{n-1}p \le \|f\|_\alpha^2 \tag{IX.49}$$

By the hypotheses, $h_p = 0$ if $|p| > \frac{1}{2}\lambda^{1/2}$. For each p with $|p| < \frac{1}{2}\lambda^{1/2}$, we define $\hat{g}_p(k) = (k^2 - (\lambda - |p|^2))^{-1}\hat{h}_p(k)$. Then, by Lemma 3,

$$|g_p(y)|^2 \le D^2\|h_p\|_\alpha^2(1 + |y|^2)^{-(\alpha - 1/2 - \varepsilon)}$$

Since

$$g_p(y) = (2\pi)^{-(n-1)/2} \int \exp\left(-i \sum_{i=1}^{n-1} p_i x_i\right)(B_\lambda f)(x_1, \ldots, x_{n-1}, y)\, d^{n-1}x$$

the Plancherel theorem and (IX.49) imply that

$$\int |(B_\lambda f)(x_1, \ldots, x_n)|^2\, d^{n-1}x \le D^2\|f\|_\alpha^2(1 + |x_n|^2)^{-(\alpha - 1/2 - \varepsilon)}$$

There are now two cases to consider. If $\alpha - 1 - 2\varepsilon \leq 0$, then

$$(1 + |x|^2)^{\alpha - 1 - 2\varepsilon} \leq (1 + |x_n|^2)^{\alpha - 1 - 2\varepsilon}$$

so

$$\|B_\lambda f\|^2_{\alpha - 1 - 2\varepsilon} \leq \int |(B_\lambda f)(x_1, \ldots, x_n)|^2 (1 + |x_n|^2)^{\alpha - 1 - 2\varepsilon}\, d^n x$$

$$\leq D^2 \|f\|^2_\alpha \int (1 + |x_n|^2)^{-1/2 - \varepsilon}\, dx_n$$

On the other hand, if $\alpha - 1 - 2\varepsilon > 0$, we must use a subtler argument. Let $\mathbf{e}_n = (0, 0, \ldots, 1)$. If $\mathbf{e}$ is a unit vector sufficiently close to $\mathbf{e}_n$, then by mimicking the above argument one can show that

$$\int |(B_\lambda f)(x_1, \ldots, x_n)|^2 (1 + |\mathbf{x} \cdot \mathbf{e}|^2)^{\alpha - 1 - 2\varepsilon}\, d^n x \leq D_1^2 \|f\|^2_\alpha \qquad \text{(IX.50)}$$

Choose unit vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ near $\mathbf{e}_n$ so that $\{\mathbf{v}_i\}_{i=1}^n$ is a basis for $\mathbb{R}^n$. Then, there is a constant C so that

$$1 + |\mathbf{x}|^2 \leq C \sum_{i=1}^n (1 + |\mathbf{x} \cdot \mathbf{v}_i|^2)$$

Thus, for some other constant C'

$$(1 + |\mathbf{x}|^2)^{\alpha - 1 - 2\varepsilon} \leq C' \sum_{i=1}^n (1 + |\mathbf{x} \cdot \mathbf{v}_i|^2)^{\alpha - 1 - 2\varepsilon}$$

Therefore by (IX.50)

$$\|B_\lambda f\|^2_{\alpha - 1 - 2\varepsilon} \leq C' D_1^2 \|f\|^2_\alpha \quad \blacksquare$$

Proof of Theorem IX.41 By a simple compactness argument we can cover $\mathbb{R}^n$ by finitely many neighborhoods $V_1, \ldots, V_m$ so that

$$V_i = \{k \mid |k - \lambda^{1/2} e_i| < \tfrac{1}{2}\lambda^{1/2}\} \qquad \text{for} \quad i = 1, 2, \ldots, m - 2$$

where $e_1, \ldots, e_{m-2}$ are unit vectors and where

$$V_{m-1} = \{k \mid |k| \leq \tfrac{3}{4}\lambda^{1/2}\}, \qquad V_m = \{k \mid |k| \geq \tfrac{5}{4}\lambda^{1/2}\}$$

Choose C^∞ functions $\{\chi_i\}_{i=1}^m$, with $\operatorname{supp} \chi_i \subset V_i$, so that $\sum_{i=1}^m \chi_i = 1$. By Lemma 1, $\sum_{i=1}^m \|\widehat{\chi_i f}\|_\alpha \leq C_1 \|f\|_\alpha$. Therefore, by Lemma 1 for $i = m - 1$ and $i = m$ and Lemma 5 for $i \leq m - 2$,

$$\|B_\lambda f\|_{\alpha - 1 - 2\varepsilon} \leq \sum_{i=1}^m \|\widehat{(k^2 - \lambda)^{-1} \chi_i \hat{f}}\|_{\alpha - 1 - 2\varepsilon} \leq C_2 \|f\|_\alpha \quad \blacksquare$$

Strč prst skrs krk *A Czech tongue-twister*

IX.10 Products of distributions, wave front sets, and oscillatory integrals

In this section we wish to discuss some results connected with the problem of defining the product of two distributions. If $T \in \mathscr{S}'(\mathbb{R}^n)$ and $S \in O_M^n$, then we have already defined ST (see Example 7 and Operation 1 in Section V.3). More singular products often occur in applications. For example, in the theory of the free quantum field, one would like to define $\theta(x-y)\Delta_+(x-y) + \theta(y-x)\Delta_+(y-x)$ where Δ_+ is the two-point function and

$$\theta(f) = \int_{x_0 \geq 0} f(x)\, d^4x$$

The problem of defining products is not to define a single product TS but to define a product with reasonable properties for a large class of T and S. In the above example, both θ and Δ_+ are singular at $x = 0$, but in a sense which we will make precise, the singularities are compatible in a way which allows us to define $\theta\Delta_+$.

We will attack the problem of products in two steps. First, we will "localize" T and S in such a way that we need consider only the case where T and S are distributions of compact support. Secondly, we will use the fact that the Fourier transform of a product is the convolution of the Fourier transforms and try to define TS so that $\widehat{TS} = (2\pi)^{-n/2}\hat{T} * \hat{S}$. This way of looking at products will lead naturally to the notion of the wave front set of a distribution. We complete the section by developing a method for computing the wave front set of a class of distributions called oscillatory integrals. Finally we use this machinery to define the product discussed above.

We remark that we will not have occasion to use the elaborate techniques of oscillatory integrals again and that they can be avoided if one merely wants to define the product $\theta\Delta_+$. We have included these techniques partly as an introduction to a set of important ideas which have found application in partial differential equations. We mention some of these applications in the Notes.

As motivation and as an introduction to localization techniques we first consider the case where T and S are singular at different points in the following precise sense:

Definition Let $T \in \mathscr{D}'(\mathbb{R}^n)$. We say that $x \in \mathbb{R}^n$ is a **regular point** of T if and only if there is a neighborhood U of x and a function F, which is C^∞ on U,

so that $T(f) = \int f(x)F(x)\,dx$ for all $f \in \mathscr{D}$ with $\operatorname{supp} f \subset U$. The complement of the regular points of T is called the **singular support** of T and will be denoted by $\operatorname{sing\,supp}(T)$.

From the definition, it is clear that:

Proposition The singular support of T is a closed subset of $\operatorname{supp} T$.

In one case, it is easy to define TS; we just localize the notion of product used in Section V.3.

Theorem IX.42 Let T and S be in $\mathscr{D}'(\mathbb{R}^n)$. Suppose that $\operatorname{sing\,supp}(T) \cap \operatorname{sing\,supp}(S) = \varnothing$. Then there is a unique $W \in \mathscr{D}'$ so that

(a) If $x \notin \operatorname{sing\,supp}(S)$ and $S = F$, a C^∞ function, near x, then $W = FT$ near x. That is, if $S(f) = \int F(x)f(x)\,dx$ for all f with $\operatorname{supp} f \subset U$, an open set about x, then $W(f) = T(Ff)$ for all f with $\operatorname{supp} f \subset U$.

(b) If $x \notin \operatorname{sing\,supp}(T)$ and $T = G$, a C^∞ function, near x, then $W = GS$ near x.

Proof Let us first prove that there is at most one such W. For suppose that W_1, W_2 satisfy (a), (b), and let f be given. Let B_R denote the ball of radius R. Since $\operatorname{sing\,supp}(T) \cap \operatorname{sing\,supp}(S) = \varnothing$, for any $x \in B_{2R}$, we can find a ball $B^{(x)}_{r(x)}$ of radius $r(x)$ about x so that $W_1(g) = W_2(g)$ for all g with $\operatorname{supp} g \subset B^{(x)}_{r(x)}$ since either (a) or (b) holds near x for both W_1 and W_2. Choose finitely many $x_1, \ldots, x_k$ in B_{2R} so that $\bigcup_{i=1}^k B^{(x_i)}_{r(x_i)/2} \supset \bar{B}_R$ and choose nonnegative $\chi_1, \ldots, \chi_k$ with

$$\chi_i \in C_0^\infty, \qquad \operatorname{supp} \chi_i \subset B^{(x_i)}_{r(x_i)}, \qquad \text{and} \qquad \chi_i \restriction B^{(x_i)}_{r(x_i)/2} \equiv 1$$

Define $h = \sum_{i=1}^k \chi_i$ and let χ be a C_0^∞ function identically one on B_R with support in N, a neighborhood of $\bar{B}_R$ on which h is bounded from below by a strictly positive constant. Then for every $f \in C_0^\infty$ with $\operatorname{supp} f \subset B_R$, we can write

$$f = f\sum_{i=1}^k \chi\chi_i h^{-1} = \sum_{i=1}^k f\chi_i h^{-1} \equiv \sum_{i=1}^k f_i$$

where $f_i = \chi_i h^{-1} f$ is C^∞ with $\operatorname{supp} f_i \subset B^{(x_i)}_{r(x_i)}$. By the above argument, $W_1(f_i) = W_2(f_i)$ so $W_1(f) = W_2(f)$. Since R was arbitrary, $W_1 = W_2$.

This proves uniqueness. Now suppose for each R we can construct a distribution W_R on $\mathscr{D}(B_R)$. Then, by the above uniqueness, the W_R must

agree on their common domain, i.e., if $R_2 > R_1$, then $W_{R_2} \restriction \mathscr{D}(B_{R_1}) = W_{R_1}$, so the W_R fit together to form a functional on $\mathscr{D}$ that is continuous since it is continuous on each $\mathscr{D}(B_R)$.

Now fix R. For each $x \in B_{2R}$, x is either a regular point for T or one for S, so pick $B^{(x)}_{r(x)}$ so that either $S \restriction B^{(x)}_{r(x)}$ is a C^∞ function F_x or $T \restriction B^x_{r(x)}$ is a C^∞ function G_x. As above, choose finitely many x_i and label them so that $x_1, \ldots, x_\ell$ have associated F's and $x_{\ell+1}, \ldots, x_k$ have associated G's. Also, as above, let $u_i = \chi\chi_i h^{-1}$ so that u_i is C^∞, $\operatorname{supp} u_i \subset B^{(x_i)}_{r(x_i)}$ and $\sum_{i=1}^k u_i = 1$ on $\bar{B}_R$. Define W_R by

$$W_R(f) = \sum_{i=1}^{\ell} T(F_{x_i} u_i f) + \sum_{i=\ell+1}^{k} S(G_{x_i} u_i f) \tag{IX.51}$$

That (IX.51) obeys (a) and (b) is left to the reader. ∎

The above procedure of defining $W(f)$ in terms of the functions $u_i f$ is known as localization. There is an important element in the above proof which implies that we do not lose anything by localization, i.e., that we can put the local pieces back together. This is the fact that the topology on $\mathscr{D}$ is defined locally, i.e., for a functional T on $\mathscr{D}$ to be continuous, we need only know that its restriction to each $\mathscr{D}(B_R)$ is continuous. This is not true of the topology on $\mathscr{S}$. In fact, one can take two tempered distributions T and S which have a product TS by Theorem IX.42 but the product is not a tempered distribution!

Example 1 Let F be the bounded C^∞ function $F(x) = \exp(ie^x)$. Since F is bounded, $F \in \mathscr{S}'$. Let F' be the distributional derivative of F. Certainly $F' \in \mathscr{S}'$. Applied to any $g \in \mathscr{D}$

$$F'(g) = \int g(x)(ie^x)F(x)\,dx \tag{IX.52}$$

although (IX.52) is not true for arbitrary $g \in \mathscr{S}$. Let $\bar{F}$ be the tempered distribution $\exp(-ie^x)$. As ordinary distributions, both $\bar{F}$ and F' have empty singular supports and so by Theorem IX.42 we can define an element W of $\mathscr{D}'$ with $W = -i\bar{F}F'$. In fact W is just e^x but e^x is not tempered (since any *positive* distribution which is tempered must be given by a polynomially bounded measure).

This example illustrates the unsuitability of localization techniques when dealing with tempered distributions. For example, F' is given locally by a C^∞ function, but it is not equal to any C^∞ function as an element of $\mathscr{S}'$.

Now we want to try to define products of distributions that may have some common singular support. The most important property of products which we want to preserve is their connection to convolutions via the Fourier transform. Of course, in general, elements $T \in \mathscr{D}'$ may not have a Fourier transform, but if we localize, i.e., consider some fT with $f \in \mathscr{D}$, then, by Theorem IX.12, $\widehat{fT}$ is an entire analytic function. Thus, we try:

Definition Let $T, S \in \mathscr{D}'$. We say that $W \in \mathscr{D}'$ is the **product** of T and S if and only if for each $x \in \mathbb{R}^n$, there exists some $f \in \mathscr{D}$, with $f = 1$ near x so that for each $k \in \mathbb{R}^n$:

$$\widehat{f^2 W}(k) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \widehat{fT}(\ell)\widehat{fS}(k-\ell)\, d\ell \tag{IX.53}$$

where the integral in (IX.53) is absolutely convergent. If such a W exists, we say the **product of T and S exists.**

Theorem IX.43

(a) The product is well defined, i.e., there is at most one W satisfying the definition.

(b) If $f \in \mathscr{D}$ and $T \in \mathscr{D}'$, then fT exists and is given by the usual definition, i.e., $fT(g) = T(fg)$.

(c) If TS, $(TS)V$, SV, and $T(SV)$ all exist, then $T(SV) = (TS)V$; if TS exists, then ST exists and $TS = ST$.

(d) If T and S are distributions with disjoint singular supports, then TS exists and is given by the product W of Theorem IX.42.

(e) If T and S are distributions of compact support, a sufficient condition that TS exist is that $\int \hat{T}(\ell)\hat{S}(k-\ell)\, d\ell$ converge absolutely for each k and define a polynomially bounded function of k.

(f) A sufficient condition for $W = TS$ to exist is that for each $x \in \mathbb{R}^n$, there is some $f \in \mathscr{D}$ with $f(x) \neq 0$ so that the integral on the right-hand side of (IX.53) converges absolutely and yields a polynomially bounded function of k.

(g) If TS exists, then $\operatorname{supp}(TS) \subset \operatorname{supp} T \cap \operatorname{supp} S$.

Proof We will prove (a) and (g) and leave the rest to the problems. We first note that if (IX.53) holds, then for any $g \in \mathscr{D}$,

$$\widehat{gf^2 W} = (2\pi)^{-n/2}\widehat{gfT} * \widehat{fS} = (2\pi)^{-n/2}\widehat{fT} * \widehat{gfS} \tag{IX.54}$$

(IX.54) follows from the associativity $\hat{g} * (\widehat{fT} * \widehat{fS}) = (\hat{g} * \widehat{fT}) * \widehat{fS}$, which is true because the necessary change of variables is legitimate on account of the assumed absolute convergence of (IX.53). Thus, if W_1 and W_2 both satisfy the definition, then for each $x \in \mathbb{R}^n$ we can find f and g identically one near x so that $\widehat{f^2 W_1} = (2\pi)^{-n/2} \widehat{fT} * \widehat{fS}$ and $\widehat{g^2 W_2} = (2\pi)^{-n/2} \widehat{gT} * \widehat{gS}$. By (IX.54), we conclude that $\widehat{f^2 g^2 W_1} = \widehat{f^2 g^2 W_2}$, so $W_1 - W_2$ vanishes near x, and thus by the argument in Theorem IX.42, it is zero.

To prove (g) we need only show that if $x \notin \operatorname{supp} T$, then $x \notin \operatorname{supp}(TS)$ and evoke symmetry. By the argument in Theorem IX.42, it is sufficient to prove that $TS(f) = 0$ for all f with support in N, some small neighborhood of x. So choose N with $T(f) = 0$ if $\operatorname{supp} f \subset N$. Then $fT \equiv 0$ since for all $g \in \mathscr{D}$, $fT(g) = T(fg) = 0$. Thus, by (c), $f(TS) = (fT)S = 0$. Finally letting χ be any function in $\mathscr{D}$ identically one on N, we have $TS(f) = TS(f\chi) = (fTS)(\chi) = 0$. ∎

Example 2 Let $T = S = \delta$ in $\mathscr{D}(\mathbb{R})$. Then $\hat{T} = \hat{S} = (2\pi)^{-1/2}$ and for any f identically one near $x = 0$, $fT = T$ so that the integral (IX.53) diverges. Thus the product TS does not exist.

Example 3 $T = S = \mathscr{P}(1/x) - i\pi\delta(x)$ where $\mathscr{P}$ is the Cauchy principle value (Example 6 of Section V.3). As we have seen (Problem 22 of Chapter V),

$$T = \lim_{\varepsilon \downarrow 0} \frac{1}{x + i\varepsilon} \tag{IX.55}$$

Using (IX.55), it is easy to show (Problem 54) that

$$\hat{T}(k) = -(2\pi)^{-1/2}(2\pi i)\theta(k) \tag{IX.56}$$

where θ is the Heavyside function given in Example 8 of Section V.3. Thus

$$\begin{aligned}(2\pi)^{-1/2} \int \hat{T}(\ell)\hat{S}(k-\ell)\, d\ell &= -(2\pi)^{-3/2}(2\pi)^2 \int \theta(\ell)\theta(k-\ell)\, d\ell \\ &= -(2\pi)(2\pi)^{-1/2} k\theta(k) \\ &= (ik)\hat{T}(k)\end{aligned}$$

Thus, by (e) of the last theorem, TS exists and $TS = -T'$; explicitly,

$$(TS)(f) = \lim_{a \downarrow 0} \int_a^\infty \left(\frac{f(x) + f(-x) - 2f(0)}{x^2} \right) dx - i\pi f'(0)$$

Example 4 There is a simple generalization of Example 3 to distributions in $\mathbb{R}^n$. Namely, if T and S have Fourier transforms with supports in a convex cone with a dual cone C having nonempty interior, then it can be shown that $\hat{T} * \hat{S}$ exists. In this case there is an alternative way of defining TS (Problem 62); for since $\hat{T}$ has support in a cone, by Theorem IX.16 there is an analytic function $\tilde{T}$ on $\mathbb{R}^n + iC$ with $T = \lim_{\kappa \downarrow 0, \kappa \in C} \tilde{T}(\cdot + i\kappa)$. Then, since $\tilde{T}$ and $\tilde{S}$ are polynomially bounded as $\kappa \to 0$, so is $\tilde{T}\tilde{S}$ so that $\lim_{\kappa \downarrow 0; \kappa \in C} \tilde{T}(\cdot + i\kappa)\tilde{S}(\cdot + i\kappa)$ exists and defines a distribution. This is identical to the TS defined by our general procedure.

In Example 3, T and S are singular at $x = 0$, but their Fourier transforms are not badly behaved in all directions. This suggests that we single out singular directions as well as singular points:

Definition Let $T \in \mathscr{D}'(\mathbb{R}^n)$. A point $\langle x, k\rangle \in \mathbb{R}^n \times (\mathbb{R}^n \backslash \{0\})$ is called a **regular directed point** for T if and only if there is a neighborhood N of x, a neighborhood M of k, and a function $g \in \mathscr{D}$, identically one in N, so that for each $m > 0$, there is a constant C_m with

$$|S(\lambda p)| \equiv |\widehat{gT}(\lambda p)| \leq C_m(1 + |\lambda|)^{-m} \tag{IX.57}$$

for all $p \in M$, $\lambda \in \mathbb{R}_+ = [0, \infty)$. The complement in $\mathbb{R}^n \times (\mathbb{R}^n \backslash \{0\})$ of the regular directed points for T is called the **wave front set** of T and denoted $WF(T)$.

Tlus $\langle x, k\rangle$ is a regular directed point if the localization gT of T near x has a Fourier transform falling off faster than any power in a cone about k (Figure IX.6).

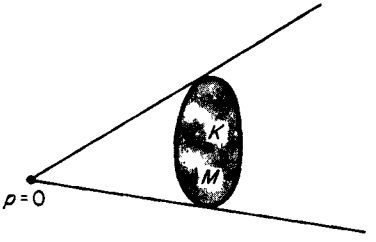


FIGURE IX.6 The cone $\bigcup_{\lambda>0} (\lambda M)$.

Theorem IX.44 Let $T \in \mathscr{D}'(\mathbb{R}^n)$. Then:

(a) $WF(T)$ is a closed subset of $\mathbb{R}^n \times (\mathbb{R}^n \backslash \{0\})$.
(b) For each $x \in \mathbb{R}^n$,

$$WF_x(T) \equiv \{k \mid \langle x, k\rangle \in WF(T)\}$$

is a cone, i.e., $k \in WF_x(T)$ and $\lambda > 0$ implies $\lambda k \in WF_x(T)$.

(c) $WF(T+S) \subset WF(T) \cup WF(S)$.

(d) $\{x \mid WF_x(T) \neq \varnothing\}$ is sing supp(T).

(e) If $T \in \mathscr{S}'$ and $\hat{T}$ has support in a closed cone C, then for each x, $WF_x(T) \subset C$.

(f) Let M be a diffeomorphism of $\mathbb{R}^n$ to $\mathbb{R}^n$ (i.e., a C^∞ map with a C^∞ inverse) and let $T \circ M$ be the distribution

$$(T \circ M)(f) = T(g^{-1}(f \circ M^{-1}))$$

where g is the determinant of the Jacobian matrix dM_x given by $(dM_x)_{ij} = \partial M_i/\partial x_j$. Let $M_* : \mathbb{R}^n \times (\mathbb{R}^n\backslash\{0\}) \to \mathbb{R}^n \times (\mathbb{R}^n\backslash\{0\})$ by

$$M_*\langle x, k\rangle = \langle M(x), dM_x^*(k)\rangle$$

where dM_x^* is the adjoint of dM_x with respect to the Euclidean inner product on $\mathbb{R}^n$. Then

$$WF(T \circ M) = M_*[WF(T)]$$

Proof (a)–(c) follow directly from the definition of $WF(T)$. For the case of linear coordinate change, (f) is easy, but in general a subtle argument is needed (Problem 75). To prove (d), we must show that x is a regular point if and only if $\langle x, k\rangle$ is a regular direction for all $k \in \mathbb{R}^n\backslash\{0\}$. The "only if" statement is clear, so suppose that $\langle x, k\rangle$ is a regular direction for each k. Then for each k in the unit sphere $S = \{k \mid |k| = 1\}$, there exist g_k, N_k, M_k so that (IX.57) holds. By the compactness of S, we can find $k_1, \ldots, k_m$ with $\bigcup_{i=1}^m M_{k_i} \supset S$. Let $g = \prod_i g_{k_i}$ and $N = \bigcap N_{k_i}$. By (IX.57) and the lemma below, $\widehat{gT}$ falls off faster than any power in each $\bigcup_{\lambda>0} \lambda \tilde{M}_{k_i}$, where $\tilde{M}_{k_i}$ is an arbitrary compact subset of M_{k_i}, and therefore in $\mathbb{R}^n\backslash\{0\}$. It follows that $\widehat{g^2T} = (2\pi)^{-n/2}\hat{g} * \widehat{gT}$ lies in $\mathscr{S}(\mathbb{R}^n)$ so that g^2T is C^∞. Since g is identically 1 near x, T is C^∞ near x.

To prove (e), choose f positive near x so that $\hat{f}$ has compact support. Then $\widehat{fT}(k) = \hat{T}(g_k)$ where $g_k(\ell) = (2\pi)^{-n/2}\hat{f}(\ell - k)$. If $k \notin C$, then for some small open set U about k, $\bar{U} \cap C = \varnothing$. For all large λ, supp $g_{\lambda\ell} \cap C = \varnothing$ for all $\ell \in U$ and so $\widehat{fT}(k)$ vanishes on λU for λ large. Now, given x, find $h \in \mathscr{D}$ so that hf is identically 1 near x. By the lemma, $\widehat{hfT}$ falls off faster than any power in $\bigcup_{\lambda>0} \lambda\tilde{U}$ where $\tilde{U}$ is a compact neighborhood of k in U. ∎

The following lemma completes the proof of Theorem IX.44.

Lemma Let M be an open set disjoint from 0 and suppose $S \in O_M^n$ obeys (IX.57) for $\lambda \in \mathbb{R}_+$, $k \in M$. Let $\tilde{M}$ be an arbitrary compact subset of M and let $h \in \mathscr{S}$. Then $h * S$ obeys (IX.57) for all $k \in \tilde{M}$, $\lambda \in \mathbb{R}_+$.

Proof Let $U = \bigcup_{\lambda>0} \lambda M$ and write

$$(S * h)\hat{}(\lambda k) = \int_{\ell \in U} S(\ell)h(\lambda k - \ell)\, d\ell + \int_{\ell \notin U} S(\ell)h(\lambda k - \ell)\, d\ell$$

On U, $|S(\ell)| \le C_m(1 + |\ell|)^{-m}$ for any m and on all of $\mathbb{R}^n$, $|h(\ell)| \le D_j(1 + |\ell|)^{-j}$ for all j. Now

$$|\lambda k| + 1 \le |\lambda k - \ell| + |\ell| + 1 \le (|\lambda k - \ell| + 1)(|\ell| + 1)$$

so that for any k,

$$\left|\int_{\ell \in U} S(\ell)h(\lambda k - \ell)\, d\ell\right| \le \int D_j C_{j+n+1}(|\lambda k| + 1)^{-j}(|\ell| + 1)^{-n-1}\, d\ell$$
$$\le (\text{const})(|\lambda k| + 1)^{-j}$$

Next let $\tilde{U} = \bigcup_{\lambda>0} \lambda \tilde{M}$ and let $\alpha = \sup\{\ell \cdot k \mid |\ell| = |k| = 1, \ell \notin U, k \in \tilde{U}\}$. Then by the compactness of $\tilde{M}$ and the openness of M, $\alpha < 1$. Thus for $\ell \notin U$, $k \in \tilde{U}$,

$$|\ell - k|^2 \ge |\ell|^2 + |k|^2 - 2\alpha|\ell||k| \ge (1 - \alpha)(|\ell|^2 + |k|^2)$$
$$\ge \tfrac{1}{2}(1 - \alpha)(|\ell| + |k|)^2$$

so $|\ell - k| \ge \beta(|\ell| + |k|)$ for suitable $\beta > 0$. Now, since $S \in O_M^n$, $|T(k)| \le E(1 + |k|^p)$ for suitable p and $|h(\ell)| \le D_{p+n+1+m}(1 + |\ell|)^{-(p+n+1+m)}$. Thus, for $k \in \tilde{U}$:

$$\left|\int_{\ell \notin U} S(\ell)h(\lambda k - \ell)\, d\ell\right| \le ED_{p+n+1+m} \int (1 + |\lambda k| + |\ell|)^{-p-n-m-1}$$
$$\times (1 + |\ell|)^p\, d\ell \le \text{const}(|\lambda k| + 1)^{-m}$$

Thus for $k \in \tilde{U}$,

$$|(S * h)\hat{}(\lambda k)| \le \text{const}(1 + |\lambda k|)^{-m}$$

Since $\inf\{|k| \mid k \in \tilde{M}\} > 0$, the lemma is proven. ∎

Example 2, revisited $WF(\delta) = \{\langle 0, \lambda\rangle \mid \lambda \neq 0\}$.

Example 3, revisited $WF(\mathscr{P}(1/x) - i\pi\delta(x)) = \{\langle 0, \lambda\rangle \mid \lambda > 0\}$.

If $\langle x, k\rangle \in WF(T)$, $\widehat{gT}$ is still polynomially bounded in direction k since gT is a tempered distribution. Thus, in "good" directions $\widehat{gT}$ falls off faster than any polynomial, while in "bad" directions it is polynomially bounded.

Thus, for any integral like $\int \widehat{gT}(\ell)\widehat{gS}(k-\ell)\,d\ell$ to converge, it is enough that each direction be good for either T or S. This suggests the following which is the first main theorem of this section:

Theorem IX.45 Let T and S be distributions. Suppose that

$$WF(T) \oplus WF(S) \equiv \{\langle x, k_1 + k_2\rangle \,\big|\, \langle x, k_1\rangle \in WF(T);\ \langle x, k_2\rangle \in WF(S)\}$$

does not contain any element of the form $\langle x, 0\rangle$. Then, the product TS exists and

$$WF(TS) \subset WF(T) \cup WF(S) \cup [WF(T) \oplus WF(S)] \qquad \text{(IX.58)}$$

Proof By definition, we need only define the product locally. So given $x \in \mathbb{R}^n$, let $\Gamma_1 = WF_x(T)$, $\Gamma_2 = WF_x(S)$. By hypothesis, $0 \notin \Gamma_1 + \Gamma_2$, so since Γ_1 and Γ_2 are closed, $\sup\{k_1 \cdot k_2 | k_1 \in \tilde{\Gamma}_1,\ -k_2 \in \tilde{\Gamma}_2\} < 1$ where we denote by $\tilde{C}$, $\{x \in C \,|\, |x| = 1\}$ for any cone C. For any closed cones K_1, K_2 in $\{\mathbb{R}^n \backslash 0\}$ with $\tilde{\Gamma}_1 \subset \tilde{K}_1^{\text{int}}$, $\tilde{\Gamma}_2 \subset \tilde{K}_2^{\text{int}}$, we can, by a compactness argument, find f identically one near x so that

$$|\widehat{fT}(k)| \le c_j(1 + |k|)^{-j} \qquad \text{all } k \notin K_1, \text{all } j \qquad \text{(IX.59)}$$

$$|\widehat{fS}(k)| \le d_j(1 + |k|)^{-j} \qquad \text{all } k \notin K_2, \text{all } j \qquad \text{(IX.60)}$$

Moreover, since fT and fS have compact support, there is an m and a D so that

$$|\widehat{fS}(k)| + |\widehat{fT}(k)| \le D(1 + |k|)^m \qquad \text{all } k \qquad \text{(IX.61)}$$

Let us suppose that K_1, K_2 are chosen so "close" to Γ_1, Γ_2 that one has

$$\beta = \sup\{k_1 \cdot k_2 \,\big|\, k_1 \in \tilde{K}_1,\ -k_2 \in \tilde{K}_2\} < 1$$

Since the corresponding sup with K_i replaced by Γ_i is less than 1, this is always possible.

We will prove that the integral

$$I(k) = \int_{\ell_2 = k - \ell_1} \widehat{fS}(\ell_1)\widehat{fT}(\ell_2)\,d\ell_1$$

converges absolutely, is polynomially bounded, and falls off faster than any power in a neighborhood of any direction $k \notin K_1 \cup K_2 \cup (K_1 + K_2)$. This will prove the existence of the product by part (e) of Theorem IX.43 and

that $WF_x(TS) \subset K_1 \cup K_2 \cup (K_1 + K_2)$. Since K_i is an arbitrarily small cone about Γ_i, we will then have $WF_x(TS) \subset \Gamma_1 \cup \Gamma_2 \cup (\Gamma_1 + \Gamma_2)$ thereby concluding the proof of the theorem.

Decompose $I(k)$ as the sum of four integrals

$$I(k) = I_1(k) + I_2(k) + I_3(k) + I_4(k)$$

over the four regions $\ell_1 \in K_1$, $\ell_2 \in K_2$; $\ell_1 \in K_1$, $\ell_2 \notin K_2$; $\ell_1 \notin K_1$, $\ell_2 \in K_2$; $\ell_1 \notin K_1$, $\ell_2 \notin K_2$. We will often use the estimate of the lemma above that

$$|x| + 1 \leq (|y| + 1)(|x - y| + 1) \tag{IX.62}$$

By (IX.59), (IX.60) and (IX.62),

$$|I_4(k)| \leq c_j d_{n+j+1} \int (|\ell_1| + 1)^{-n-j-1}(|\ell_1 - k| + 1)^{-j}\, d\ell_1$$

$$\leq (|k| + 1)^{-j}\left[c_j d_{n+j+1} \int (|\ell_1| + 1)^{-n-1}\, d\ell_1\right]$$

so the integral in I_4 converges and falls off faster than any power in all directions.

Now $I_1(k) = 0$ unless $k \in K_1 + K_2$ so we need only prove the convergence of the integral and its polynomial boundedness to control the contribution of I_1, for it is automatic that $WF(I_1) \subset K_1 + K_2$. Now, if $\ell_1 \in K_1$, $\ell_2 \in K_2$, then

$$|\ell_1 + \ell_2|^2 \geq \tfrac{1}{2}(1 - \beta)(|\ell_1| + |\ell_2|)^2$$

Thus, for fixed k, the only ℓ's that enter in the integral I_1 have $|\ell_1|$, $|\ell_2| \leq 2(1 - \beta)^{-1}|k|$. Using (IX.61), we see that $I_1(k)$ converges and

$$I_1(k) \leq \int_{|\ell_1| \leq 2(1-\beta)^{-1}|k|} D^2[1 + 2(1 - \beta)^{-1}|k|]^{2m}\, d\ell_1$$

$$= D^2[1 + 2(1 - \beta)^{-1}|k|]^{2m+n} \times (\text{volume of unit ball})$$

Finally we consider I_2; the proof for I_3 is similar. By (IX.61) and (IX.60):

$$I_2(k) \leq D d_{j+m+n+1} \int_{k-\ell_2 \in K_1} (1 + |k - \ell_2|)^m (1 + |\ell_2|)^{-j-m-n-1}\, d\ell_2$$

If we ignore the $k - \ell_2 \in K_1$ condition and use $|k - \ell_2| \leq |k| + |\ell_2|$, we see that the integral converges and is polynomially bounded. We also claim that $I_2(k_0)$ falls off polynomially if $k_0 \notin K_1$, so that $WF(I_2) \subset K_1$. For if

$k_0 \notin K_1$, choose a cone K_3 about k_0 so that $\sup\{k_1 \cdot k_2 | k_1 \in \tilde{K}_1, k_2 \in \tilde{K}_3\} = \gamma < 1$. Then for $k \in K_3$, $k - \ell_2 \in K_1$, we have $|\ell_2| \geq \frac{1}{2}(1-\gamma)(|k| + |k-\ell_2|)$, so that for $k \in K_3$,

$$I_2(k) \leq Dd_{j+m+n+1} \int (1 + |\ell_1|)^m [1 + \tfrac{1}{2}(1-\gamma)(|k| + |\ell_1|)]^{-j-m-n-1} \, d\ell_1$$

$$\leq \text{const}(1 + |k|)^{-j}$$

Thus $WF(I_2) \subset K_1$. By Theorem IX.44c,

$$WF(I) \subset \bigcup_{j=1}^{4} WF(I_j) \subset (K_1 + K_2) \cup K_1 \cup K_2 . \blacksquare$$

Example 3, yet again $WF(\mathscr{P}(1/x) - i\pi\delta(x)) = \{\langle 0, \lambda\rangle | \lambda > 0\}$. Thus, by Theorem IX.45, all powers of $\mathscr{P}(1/x) - i\pi\delta(x)$ exist.

Example 5 Let x_1 and x_2 be the coordinates in $\mathbb{R}^2$ and let $\delta(x_1)$, $\delta(x_2)$ be defined in the usual way, e.g.

$$\int f(x_1, x_2)\delta(x_1)\, dx_1\, dx_2 = \int f(0, x_2)\, dx_2$$

Then

$$WF(\delta(x_1)) = \{\langle 0, x_2; \lambda, 0\rangle \,\big|\, x_2 \in \mathbb{R}, \lambda \neq 0\}$$

$$WF(\delta(x_2)) = \{\langle x_1, 0; 0, \lambda\rangle \,\big|\, x_1 \in \mathbb{R}, \lambda \neq 0\}$$

By the theorem, $\delta(x)\delta(y)$ exists and is clearly $\delta(x_1, x_2)$, the distribution taking f into $f(0)$.

To employ the machinery we have developed, one needs a method for computing wave front sets. We consider first a special example which we will then generalize sufficiently to compute the wave front set of the two-point function $\Delta_+(x; m^2)$ for a free quantum field.

Example 6 Let T_α be the Fourier transform of $(2\pi)^{-1/2}(1 + |k|^2)^\alpha$ in $\mathscr{S}'(\mathbb{R})$. If α is a positive integer n, then

$$T_n = \sum_{m=0}^{n} (-1)^m \binom{n}{m} \delta^{(2m)}(x)$$

clearly has support at zero with $WF(T_n) = \{\langle 0, \lambda\rangle \mid \lambda \neq 0\}$. One can also compute T_{-1} explicitly by a contour integration:

$$T_{-1}(x) = (2\pi)^{-1} \int_{-\infty}^{\infty} e^{-ikx}(1 + k^2)^{-1}\, dk$$
$$= \tfrac{1}{2}e^{-|x|}$$

and more generally any T_{-n}. T_{-1} does not have $\{0\}$ as support, but it does have it as singular support. This suggests that, in general, T_α might have $\{0\}$ as singular support. How might we show this? If T_α is C^∞ away from zero, then we would expect $x^n T_\alpha$ to be *globally* smoother and smoother as n gets larger and larger. Moreover, if we can show for any m, there is an n with $x^n T_\alpha \in C^m(\mathbb{R})$, then clearly T_α is C^∞ away from zero. But

$$\widehat{x^n T_\alpha} = \left(i\frac{d}{dk}\right)^n \hat{T}_\alpha \equiv f_{\alpha, n}$$

where, by explicit computation

$$|f_{\alpha, n}(k)| \leq C(1 + k^2)^{\alpha - n/2}$$

Thus, for any fixed α and m we can find n with $k^m f_{\alpha, n}(k) \in L^1$ (e.g. $n > m + 2\alpha + \frac{1}{2}$) and so T_α is C^∞ away from $x = 0$. Finally one can see that T_α is not smooth near zero. For by the Paley–Wiener idea and the fact that $(1 + k^2)^\alpha$ is analytic in the strip $|\operatorname{Im} k| < 1$, T_α and its derivatives all fall off exponentially. If T_α were C^∞ at zero, T_α and thus $\hat{T}_\alpha$ would be in $\mathscr{S}$.

What was essential in the above argument was that all the derivatives of $\hat{T}_\alpha$ fall off faster and faster, i.e., that it not behave like $x^{-n}\sin x$ whose derivatives are asymptotic to $\pm x^{-n}\sin x$ or $\pm x^{-n}\cos x$ at infinity. We thus define:

Definition *A* C^∞ function F on $\mathbb{R}^n$ is called a **symbol of order** k on $\{0\} \times \mathbb{R}^n$ if and only if for all $\alpha \in I_+^n$, there is a d_α with

$$|(D^\alpha F)(x)| \leq d_\alpha(1 + |x|)^{(k - |\alpha|)}$$

A distribution F on $\mathbb{R}^n$ is called an **approximate symbol of order** k on $\{0\} \times \mathbb{R}^n$ if and only if, for any $\alpha \in I_+^n$, there exists a compact set S_α and a constant d_α so that F is equal to a $C^{|\alpha|}$ function outside S_α which satisfies

$$|(D^\alpha F)(x)| \leq d_\alpha(1 + |x|)^{(k - |\alpha|)}$$

The phrase "on $\{0\} \times \mathbb{R}^n$" is included since this will be a special case of a definition to appear shortly. For the present, we suppress the phrase "on $\{0\} \times \mathbb{R}^n$."

Theorem IX.46 Let F be an approximate symbol of order k. Let $T = \hat{F}$. Then the singular support of T is either empty or $\{\langle 0, \ldots, 0\rangle\}$.

Proof The proof using the basic idea of Example 6 is left to the reader (Problem 66).

The above theorem does not cover many examples of interest: for example, we recall that $\Delta_+(x; m^2)$ has the form

$$\Delta_+(x; m^2) = \frac{i}{2(2\pi)^3} \int \exp(i\psi(x, k)) \frac{d^3k}{\sqrt{m^2 + k^2}}$$

with $\psi(x, k) = -x_0\sqrt{m^2 + k^2} + \mathbf{x} \cdot \mathbf{k}$. This is something like the examples given in Theorem IX.46 but the phase factor is more complicated than $ik \cdot x$ and the integration variables are fewer than in the Fourier transform. We thus introduce a larger class of examples:

Definition Let Ω be an open set in $\mathbb{R}^n$. A function $a(\cdot, \cdot)$: $\Omega \times \mathbb{R}^s \to \mathbb{C}$ is called a **symbol of order** m on $\Omega \times \mathbb{R}^s$ if and only if, for each compact $K \subset \Omega$ and $\alpha \in I_+^n$, $\beta \in I_+^s$, there is a constant $d_{\alpha, \beta, K}$ with

$$|(D_x^\alpha D_\theta^\beta a)(x, \theta)| \leq d_{\alpha, \beta, K}(1 + |\theta|)^{m - |\beta|} \tag{IX.63}$$

for all $x \in K$, $\theta \in \mathbb{R}^s$. The family of all symbols of order m with the seminorms

$$\|a\|_{\alpha, \beta, K} = \sup_{x \in K, \theta} (1 + |\theta|)^{|\beta| - m} |(D_x^\alpha D_\theta^\beta a)(x, \theta)|$$

will be denoted by $\mathrm{Sym}(\Omega, s, m)$.

We say that $a(\cdot, \cdot)$: $\Omega \times \mathbb{R}^s \to \mathbb{C}$ is an **asymptotic symbol of order** m **on** $\Omega \times \mathbb{R}^s$ if and only if $a = a_1 + a_2$ with $a_1 \in \mathrm{Sym}(\Omega, s, m)$ and where (i) a_2 has compact support in the θ variables and (ii) the map $x \to a_2(x, \cdot)$ is C^∞ as a map from Ω to $L^\infty(\mathbb{R}^s)$.

Definition A **phase function** on $\Omega \times \mathbb{R}^s$ is a function φ: $\Omega \times \mathbb{R}^s \to \mathbb{R}$ such that

(i) φ is continuous and homogeneous of degree 1 in θ, i.e., $\varphi(x, \lambda\theta) = \lambda\varphi(x, \theta)$ for all $\langle x, \theta\rangle \in \Omega \times \mathbb{R}^s$ and $\lambda \geq 0$;

(ii) φ is C^∞ on $\Omega \times (\mathbb{R}^s \backslash \{0\})$;
(iii) φ has no critical points in $\Omega \times (\mathbb{R}^s \backslash \{0\})$, i.e., the $\mathbb{R}^n \times \mathbb{R}^s$-valued function $\langle \operatorname{grad}_x \varphi, \operatorname{grad}_\theta \varphi \rangle$ is never zero.

Definition An **oscillatory integral on** $\Omega \times \mathbb{R}^s$ is a formal expression

$$\int_{\theta \in \mathbb{R}^s} e^{i\varphi(x,\theta)} a(x, \theta)\, d\theta$$

where φ is a phase function and a is an asymptotic symbol.

Example 7 We can write

$$\Delta_+(x; m^2) = \frac{i}{2(2\pi)^3} \int e^{i\varphi(x,\theta)} a(x, \theta; m)\, d\theta$$

where

$$\varphi(x, \theta) = -x_0|\theta| + \mathbf{x} \cdot \boldsymbol{\theta}$$
$$a(x, \theta; m) = (m^2 + |\theta|^2)^{-1/2} \exp(-ix_0[(m^2 + |\theta|^2)^{1/2} - |\theta|])$$

Let $\Omega = \mathbb{R}^4$. Clearly φ is a phase function since $\partial\varphi/\partial x_0 = |\theta| \neq 0$ if $\langle x, \theta \rangle \in \mathbb{R}^4 \times (\mathbb{R}^3 \backslash \{0\})$. The function a is not C^∞ because $|\theta|$ is not smooth at $\theta = 0$, but using $\left|\sqrt{m^2 + \theta^2} - |\theta|\right| \leq C(|\theta| + 1)^{-1}$, it is not hard to prove that a is an asymptotic symbol of order -1 (Problem 68). For example, let us show that $\partial a/\partial\theta_i$ falls off like $|\theta|^{-2}$ (for θ large). Let $f = (m^2 + \theta^2)^{-1/2}$ and $g = [(m^2 + |\theta|^2)^{1/2} - |\theta|.]$ Then

$$\left|\frac{\partial f}{\partial \theta_i}\right| = \left|\frac{\theta_i}{\theta}\right| \left|\frac{\theta}{(m^2 + \theta^2)^{-3/2}}\right| \leq c|\theta|^{-2} \qquad \text{for } \theta \text{ large}$$

and

$$\left|\frac{\partial g}{\partial \theta_i}\right| = \left|\frac{\theta_i}{\theta}\right| |[(m^2 + |\theta|^2)^{-1/2}\theta - 1]|$$
$$\leq [(1 + m^2|\theta|^{-2})^{-1/2} - 1] \leq c|\theta|^{-2}$$

Thus

$$\left|\frac{\partial a}{\partial \theta_i}\right| \leq \left|\frac{\partial f}{\partial \theta_i}\right| + \left|x_0 f \frac{\partial g}{\partial \theta_i}\right| \leq c|\theta|^{-2}$$

Since a is an asymptotic symbol, Δ_+ is an oscillatory integral.

We are heading toward a general theorem which will tell us that any oscillatory integral defines a distribution in a natural way and which identifies the wave front set of the distribution so defined. We first note two simple facts without proof (Problem 69):

Lemma 1 The C^∞ functions of compact support in $\Omega \times \mathbb{R}^s$ are dense in $\mathrm{Sym}(\Omega, s, m)$ in the topology of $\mathrm{Sym}(\Omega, s, m')$ whenever $m' > m$. In particular, a map from the functions of compact support to a topological space has at most one continuous extension to $\bigcup_{m<\infty} \mathrm{Sym}(\Omega, s, m)$ continuous on each $\mathrm{Sym}(\Omega, s, m)$ in its natural topology.

Lemma 2 Let $a(x, \theta)$ be a function of compact support in $\Omega \times \mathbb{R}^s$ so that $x \to a(x, \theta)$ is C^∞ as an L^∞-valued function on Ω. Then, for any phase function, $\int a(x, \theta) e^{i\varphi(x,\theta)}\, d\theta$ is a C^∞ function of x.

For the main theorem, we will need to define and develop one more concept:

Definition Let $\varphi(x, \theta)$ be a phase function on $\Omega \times \mathbb{R}^s$ where Ω is an open set in $\mathbb{R}^n$. Let

$$M(\varphi) = \{\langle x, \theta\rangle \in \Omega \times \mathbb{R}^s \backslash \{0\} \mid (\nabla_\theta \varphi)(x, \theta) = 0\}$$

$$SP(\varphi) = \{\langle x, (\nabla_x \varphi)(x, \theta)\rangle \mid \langle x, \theta\rangle \in M(\varphi)\} \subset \Omega \times \mathbb{R}^n$$

$SP(\varphi)$ is called **the manifold of stationary phase for** φ.

Lemma 3 $SP(\varphi)$ is a *closed* subset of $\Omega \times (\mathbb{R}^n \backslash \{0\})$ and if $\langle x, k\rangle \in SP(\varphi)$, then $\langle x, \lambda k\rangle \in SP(\varphi)$ for all $\lambda > 0$.

Proof Since φ is a phase function, it has no critical points so if $\langle x, \theta\rangle \in M(\varphi)$, then $\nabla_x \varphi \neq 0$. Thus $SP(\varphi) \subset \Omega \times (\mathbb{R}^n \backslash \{0\})$. If $\langle x, \theta\rangle \in SP(\varphi)$, then $\langle x, \lambda\theta\rangle \in SP(\varphi)$ since φ is homogeneous of degree one so that $(\nabla_x \varphi)(x, \lambda\theta) = \lambda(\nabla_x \varphi)(x, \theta)$. Finally, since $M(\varphi)$ is the set of zeros of a continuous function, it is closed. By a simple argument $\{x \mid M_x(\varphi) \neq \varnothing\}$ is closed. Since $\nabla_x \varphi$ is continuous, $SP(\varphi)$ is closed as the graph of a continuous function on a closed set. ∎

Example 7, continued $\varphi(x, \theta) = -x_0|\theta| + \mathbf{x} \cdot \boldsymbol{\theta}$. Thus

$$\nabla_\theta \varphi = -x_0 \boldsymbol{\theta} |\theta|^{-1} + \mathbf{x}$$

so

$$M(\varphi) = \{\langle x, \theta\rangle \mid x = 0\} \cup \{\langle x, \theta\rangle \mid |\mathbf{x}| = |x_0| \neq 0; \boldsymbol{\theta} = \lambda \mathbf{x}/x_0 \text{ with } \lambda > 0\}$$

Since $\nabla_x \varphi(x, \theta) = \langle -|\theta|, \boldsymbol{\theta}\rangle$ we conclude that

$$SP(\varphi) = \{\langle 0, 0; -|\theta|, \boldsymbol{\theta}\rangle | \boldsymbol{\theta} \in \mathbb{R}^3\}$$
$$\cup \{\langle \pm|\mathbf{x}|, \mathbf{x}; -\lambda|\mathbf{x}|, \mp\lambda\mathbf{x}\rangle | \mathbf{x} \in \mathbb{R}^3 \quad \text{and} \quad \lambda > 0\}$$

Thus $\{x \mid SP_x(\varphi) \neq \varnothing\}$ is the light cone $\{x \mid x_0 = \pm|\mathbf{x}|\}$, and $SP(\varphi)$ is the family of tangent vectors to the light cone which are lightlike and have negative time component (see Figure IX.7).

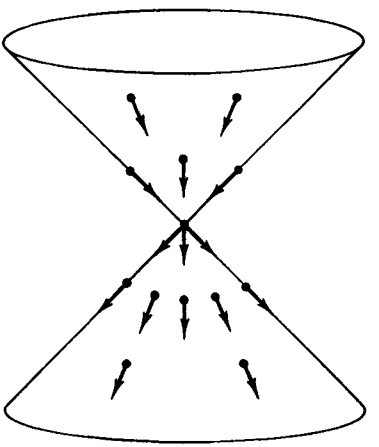


FIGURE IX.7 The set $SP(\varphi)$.

We come now to the second main theorem of this section.

Theorem IX.47 Let $\Omega \subset \mathbb{R}^n$ be a fixed open set and let $\varphi(x, \theta)$ be a fixed phase function on $\Omega \times \mathbb{R}^s$. Then, with each asymptotic symbol a on $\Omega \times \mathbb{R}^s$, we can associate a distribution $D_\varphi(a)$ on Ω so that:

(a) $a \to D_\varphi(a)$ is a linear map.
(b) If a has compact support in θ, then $D_\varphi(a)$ is the C^∞ function

$$\int_{\theta \in \mathbb{R}^s} a(x, \theta) e^{i\varphi(x, \theta)}\, d\theta$$

(c) The restriction of $D_\varphi(\cdot)$ to $\mathrm{Sym}(\Omega, s, m)$ is a continuous function from $\mathrm{Sym}(\Omega, s, m)$ to $\mathscr{D}'_\Omega$.

D_φ is uniquely determined by (a)-(c) and moreover:

(d) For any asymptotic symbol a, $WF(D_\varphi(a)) \subset SP(\varphi)$, the manifold of stationary phase for φ.

$D_\varphi(a)$ is denoted by the formal expression

$$D_\varphi(a) = \int a(x, \theta) e^{i\varphi(x,\theta)}\, d\theta$$

The main element of the proof is the development and exploitation of an "integration-by-parts" machine generalizing the fact $-ix^{-1}(d/dk)e^{ikx} = e^{ikx}$ used in analyzing Example 6:

Lemma 4 Let φ be a phase function on $\Omega \times \mathbb{R}^s$ with $\Omega \subset \mathbb{R}^n$. Then there exist functions $a_1, \ldots, a_s, b_1, \ldots, b_n$, and c on $\Omega \times \mathbb{R}^s$ so that

(1) $a_i \in \mathrm{Sym}(\Omega, s, 0)$; $i = 1, \ldots, s$
(2) $b_j \in \mathrm{Sym}(\Omega, s, -1)$; $j = 1, \ldots, n$
(3) $c \in \mathrm{Sym}(\Omega, s, -1)$
(4) ${}^tVe^{i\varphi} = e^{i\varphi}$

where V is the differential operator

$$V = \sum_{j=1}^{s} a_j \frac{\partial}{\partial \theta_j} + \sum_{k=1}^{n} b_k \frac{\partial}{\partial x_k} + c$$

and ${}^tV$ is its adjoint

$${}^tVf = -\sum_{j=1}^{s} \frac{\partial}{\partial \theta_j}(a_j f) - \sum_{k=1}^{n} \frac{\partial}{\partial x_k}(b_k f) + cf$$

Proof Since φ has no critical points on $\Omega \times (\mathbb{R}^s \backslash \{0\})$, the function $\eta(x, \theta)$ given by

$$\eta(x, \theta) = \sum_{k=1}^{n} \left(\frac{\partial \varphi}{\partial x_k}\right)^2 + |\theta|^2 \sum_{j=1}^{s} \left(\frac{\partial \varphi}{\partial \theta}\right)^2$$

is nonvanishing on $\Omega \times (\mathbb{R}^s \backslash \{0\})$. Moreover, since φ is homogeneous of order 1 in θ, η is homogeneous of order 2, i.e., $\eta(x, \lambda\theta) = \lambda^2 \eta(x, \theta)$. Let $\chi(\theta)$ be a function in $C_0^\infty(\mathbb{R}^s)$ identically one near $\theta = 0$ and let

$$\tilde{a}_j = -i(1 - \chi)\eta^{-1}|\theta|^2 \frac{\partial \varphi}{\partial \theta_j}$$

$$\tilde{b}_k = -i(1 - \chi)\eta^{-1} \frac{\partial \varphi}{\partial x_j}$$

$$\tilde{c} = \chi$$

Let $U = \sum_j \tilde{a}_j \partial/\partial\theta_j + \sum_k \tilde{b}_k \partial/\partial x_k + \tilde{c}$. Then $Ue^{i\varphi} = -i(1-\chi)\eta^{-1}(\eta ie^{i\varphi}) + \chi e^{i\varphi} = e^{i\varphi}$. Moreover $\tilde{a}_j, \tilde{b}_k$ are C^∞ functions which are homogeneous in θ near $\theta = \infty$ (e.g., $\tilde{a}_j(\lambda\theta, x) = \tilde{a}_j(\theta, x)$ if $\lambda > 1$, $\theta >$ radius of supp χ). As a result the derivatives of $\tilde{a}_j$ and $\tilde{b}_k$ are homogeneous near infinity in just the right way to guarantee that $\tilde{a}_j \in \mathrm{Sym}(\Omega, s, 0)$ and $\tilde{b}_k \in \mathrm{Sym}(\Omega, s, -1)$. Clearly $\tilde{c} \in \mathrm{Sym}(\Omega, s, -1)$. Letting $a_j = -\tilde{a}_j, b_j = -\tilde{b}_j, c = \tilde{c} - \sum_{j=1}^s \partial a_j/\partial\theta_j - \sum_{k=1}^n \partial b_k/\partial x_k$, the lemma is proven. ∎

Proof of Theorem IX.47 Let a be an asymptotic symbol and write $a = a_1 + a_2$ where a_1 has compact support and a_2 is a symbol. Then $D_\varphi(a_1)$ is determined by (b) and is C^∞ by Lemma 2. Moreover, if we can construct $D_\varphi(a_2)$ obeying (b) and (c), it is uniquely determined by Lemma 1.

We claim we are thus reduced to proving that $D_\varphi(a)$ defined by (b) extends continuously to $\bigcup_{m>0} \mathrm{Sym}(\Omega, s, m)$ (in the sense of (c)) and that for any symbol a, $WF(D_\varphi(a)) \subset SP(\varphi)$. For, if $WF(T) = \varnothing$, then $WF(T+S) \subset WF(S)$ and $WF(S) = WF(T+S-S) \subset W(T+S)$ so $WF(D_\varphi(a_1)) = \varnothing$ implies that $WF(D_\varphi(a)) = WF(D_\varphi(a_2)) \subset SP(\varphi)$.

Now, let a have compact support in $\Omega \times \mathbb{R}^s$ and be C^∞. Let $D_\varphi(a)$ be the distribution given by the C^∞ function $\int a(x,\theta)e^{i\varphi(x,\theta)}\,d\theta$. Fix $f \in \mathscr{D}_\Omega$. Then, for any integer p,

$$[D_\varphi(a)](f) = \int a(x,\theta)e^{i\varphi(x,\theta)}f(x)\,dx\,d\theta$$

$$= \int [({}^tV)^p e^{i\varphi(x,\theta)}]a(x,\theta)f(x)\,dx\,d\theta$$

$$= \int e^{i\varphi(x,\theta)}V^p(a(x,\theta)f(x))\,dx\,d\theta$$

so

$$|[D_\varphi(a)](f)| \le \int |V^p(a(x,\theta)f(x))|\,dx\,d\theta$$

Now, it is easy to see that $\langle a, f\rangle \mapsto af$ is a continuous bilinear map of $\mathrm{Sym}(\Omega, s, m) \times C_0^\infty(\Omega) \to \mathrm{Sym}(\Omega, s, m)$ and that V is a continuous map of $\mathrm{Sym}(\Omega, s, m)$ to $\mathrm{Sym}(\Omega, s, m-1)$ (Problems 70, 71). Thus $V^p(a(x,\theta)f(x))$ is a compactly supported symbol of order $m-p$ and, in particular,

$$|V^p(a(x,\theta)f(x))| \le |||a|||_p \|f\|_p (1+|\theta|)^{m-p}$$

for suitable norms $|||\cdot|||_p$ and $\|\cdot\|_p$ on $\mathrm{Sym}(\Omega, s, m)$ and $C_0^\infty(K)$ (support $f \subset K \subset \Omega$; K compact). Fixing $p > n+m$,

$$|D_\varphi(a)(f)| \le C_{p,K}|||a|||_p \|f\|_p$$

where $C_{p,K}$ is a constant only dependent on K and p. Thus the map $a \to D_\varphi(a)$ from $C_0^\infty(\Omega \times \mathbb{R}^s)$ to $\mathscr{D}'_\Omega$ extends to a continuous map from $\mathrm{Sym}(\Omega, s, m)$ to $\mathscr{D}'_\Omega$.

All that remains is to prove that $WF(D_\varphi(a)) \subset SP(\varphi)$ for any $a \in \mathrm{Sym}(\Omega, s, m)$. To do this, we must develop our machinery a little further:

Lemma 5 Let M be an open set in Ω and C a cone in $\mathbb{R}^n\backslash\{0\}$ so that $M \times C$ is disjoint from $SP(\varphi)$. Then there exist functions $A_1, \ldots, A_s$, $B_1, \ldots, B_n$ and D on $M \times C \times (\mathbb{R}^s\backslash\{0\})$ so that:

(a) A_i, B_j, and D are C^∞ on $M \times C \times (\mathbb{R}^s\backslash\{0\})$ and homogeneous of degree -1 *jointly* in $\langle k, \theta\rangle$, i.e., $A_i(x, \lambda k, \lambda\theta) = \lambda^{-1} A_i(x, k, \theta)$, etc.

(b) ${}^tV_k \exp(i\tilde{\varphi}) = \exp(i\tilde{\varphi})$ where

$$V_k = \sum_{j=1}^{s} A_j(x, k, \theta)|\theta| \frac{\partial}{\partial \theta_j} + \sum_{\ell=1}^{n} B_\ell(x, k, \theta) \frac{\partial}{\partial x_\ell} + D$$

and

$$\tilde{\varphi}(x, k, \theta) = \varphi(x, \theta) - k \cdot x$$

Proof Let

$$\tilde{\eta}(x, \theta, k) = |\theta|^2 \sum_{j=1}^{s} \left(\frac{\partial \varphi}{\partial \theta}\right)^2 + \sum_{\ell=1}^{n} \left(\frac{\partial \varphi}{\partial x_\ell} - k_\ell\right)^2$$

Then, by the definition of $SP(\varphi)$, $\tilde{\eta}$ is nonvanishing on $M \times [C \times (\mathbb{R}^s\backslash\{0\})]$. Define

$$A_j = +i\tilde{\eta}^{-1}|\theta| \frac{\partial \varphi}{\partial \theta_j}$$

$$B_\ell = +i\tilde{\eta}^{-1}\left(\frac{\partial \varphi}{\partial x_\ell} - k_\ell\right)$$

$$C = \sum_{j=1}^{s} \frac{\partial(|\theta| A_j)}{\partial \theta_j} + \sum_{k=1}^{n} \frac{\partial B_k}{\partial x_k}$$

Since $\tilde{\eta}$ is nonvanishing on $M \times C \times (\mathbb{R}^s\backslash\{0\})$ and homogeneous of degree 2 in $\langle k, \theta\rangle$ the lemma follows as in Lemma 3. ∎

Conclusion of the Proof of Theorem IX.47 Suppose $\langle x_0, k_0\rangle \notin SP(\varphi)$. Choose a neighborhood of $\langle x_0, k_0\rangle$, $M \times C$, as in Lemma 5. Let χ be a $C_0^\infty(\mathbb{R}^n)$ function with support in M identically one near x_0. For each

pair of positive integers m, n, we will find a continuous norm $|||\cdot|||_{(m,n)}$ on $\mathrm{Sym}(\Omega, s, m)$ so that

$$|\widehat{\chi D_\varphi(a)}(k)| \leq |||a|||_{(m,n)}(1 + |k|)^{-n} \qquad \text{for all } k \in C \qquad \text{(IX.64)}$$

for any $a \in C_0^\infty(\Omega \times \mathbb{R}^s)$. By the continuity we have already proven, (IX.64) will extend to all $a \in \mathrm{Sym}(\Omega, s, m)$ thus proving that $\langle x_0, k_0\rangle \notin WF(D_\varphi(a))$. Choose $\psi(\theta)$ in $C_0^\infty(\mathbb{R}^s)$, identically one if $|\theta| < 1$ and identically zero if $|\theta| > 2$. Write $a = \psi a + (1 - \psi)a$. By Lemma 2, $\widehat{\chi D_\varphi(\psi a)}(k)$ obeys an estimate of the form (IX.64). For $k \in C$, write

$$\begin{aligned}
|\widehat{\chi D_\varphi((1-\psi)a)}(k)| &= \left| \int \exp(i\tilde{\varphi}(x, k, \theta))\chi(x)(1 - \psi(\theta))a(x, \theta)\, dx\, d\theta \right| \\
&= \left| \int \exp(i\tilde{\varphi}(x, k, \theta)) V_k^p[\chi(x)a(x, \theta)(1 - \psi(\theta))]\, dx\, d\theta \right| \\
&\leq \int |V_k^p[\chi a(1 - \psi)]|\, dx\, d\theta \qquad \text{(IX.65)}
\end{aligned}$$

We claim that $|V_k^p[\chi a(1 - \psi)]| \leq |||a|||(|k| + |\theta|)^{-p}(1 + |\theta|)^m$, where $|||\cdot|||$ is a norm on $\mathrm{Sym}(\Omega, s, m)$, on account of the homogeneity properties of A, B, D in $\langle k, \theta\rangle$. Since $1 - \psi$ vanishes if $|\theta| < 1$, for all θ in the integral (IX.65), we can use

$$\begin{aligned}
(|k| + |\theta|)^{-1} &\leq (|k| + 1)^{-1} \\
(|k| + |\theta|)^{-1} &\leq (|\theta|)^{-1} \leq (\tfrac{1}{2} + \tfrac{1}{2}|\theta|)^{-1}
\end{aligned}$$

and so obtain (IX.64) by taking p sufficiently large and using the fact that the χ factor makes the x integration in (IX.65) finite. ∎

* * *

Throughout this chapter, we have developed various techniques for using the Fourier transform to analyze functions or distributions. Now, we can use these methods to analyze the distribution $\Delta_+(x, m^2)$.

Theorem IX.48 The two-point function $\Delta_+(x, m^2)$ of the free field has the following properties:

(a) Δ_+ is Lorentz invariant.

(b) $WF(\Delta_+) = \{\langle 0, 0; -|\theta|, \theta\rangle \mid \theta \in \mathbb{R}^3\}$
$\cup \{\langle \pm|\mathbf{x}|, \mathbf{x}, -\lambda|\mathbf{x}|, \mp\lambda\mathbf{x}\rangle \mid \mathbf{x} \in \mathbb{R}^3, \lambda > 0\}$

(c) There exist C^∞ functions f_s, f_t^+, and f_t^- on $(0, \infty)$ so that

$$\Delta_+(x; m^2) = \begin{cases} f_s(x^2; m^2) & \text{if } x^2 < 0 \\ f_t^+(x^2; m^2) & \text{if } x^2 > 0, x_0 > 0 \\ f_t^-(x^2; m^2) & \text{if } x^2 > 0, x_0 < 0 \end{cases}$$

where $x^2 = x \cdot \tilde{x} = x_0^2 - x_1^2 - x_2^2 - x_3^2$.

(d) For $y > 1, f_s(y^2) \leq C_\varepsilon \exp(-(m - \varepsilon)y)$.

(e) $\lim_{y \to \infty} |y|^{2n} f_t^{\pm}(y) = 0$.

(f) $f_t^+(y) = \overline{f_t^-(y)}$.

Proof (a) follows from the fact that Δ_+ is the Fourier transform of a Lorentz invariant measure. To prove (b) we note that, by our analysis of Example 7 and Theorem IX.47, $WF(\Delta_+)$ is contained in the set $S_0 \cup S_+ \cup S_-$ where $S_0 = \{\langle 0, 0, -|\theta|, \theta\rangle | \theta \in \mathbb{R}^3\}; S_\pm = \{\langle \pm|\mathbf{x}|, \mathbf{x}, -\lambda|\mathbf{x}|, \mp\lambda\mathbf{x}\rangle | \mathbf{x} \in \mathbb{R}^3, \mathbf{x} \neq \mathbf{0}, \lambda > 0\}$. Moreover, since Δ_+ is Lorentz invariant, $WF(\Delta_+)$ must be Lorentz invariant which means that S_+ is either contained in $WF(\Delta_+)$ or disjoint from it. If S_+ were disjoint from $WF(\Delta_+)$, then Δ_+ would equal a C^∞ function on $\{\langle t, \mathbf{x}\rangle | t > 0\}$. Since we will see that $\Delta_+(t_0, \mathbf{x})$ and its derivatives fall off exponentially as $\mathbf{x} \to \infty$ with t_0 fixed, it would follow that for $t_0 > 0$ $\Delta_+(t_0, \cdot)$ was in $\mathscr{S}(\mathbb{R}^3)$. Since its Fourier transform is not even L^1, S_+ cannot be disjoint from $WF(\Delta_+)$. By (f), once we know that $S_+ \subset WF(\Delta_+)$, we can conclude that $S_- \subset WF(\Delta_+)$. Finally, since $WF(\Delta_+)$ is closed and $S_0 \subset \overline{S}_+$, we have $S_0 \subset WF(\Delta_+)$. (b) implies that the singular support of Δ_+ is $\{x | x^2 = 0\}$ so Δ_+ is C^∞ in the regions in question and Lorentz invariant. This proves (c).

To prove (d), consider the distribution on $\mathbb{R}^3$ whose Fourier transform is $(k^2 + m^2)^{-1/2}$. By the Paley-Wiener idea (Problem 76) and the fact that $(k^2 + m^2)^{-1/2}$ is analytic in a tube, this distribution falls off exponentially with any exponent $a < m - \varepsilon$. Since $\Delta_+(0, x)$ is this distribution (up to a constant) we have proven (d).

To prove (e), we note that formally

$$f_t^+(x^2; m^2) = \frac{i}{2(2\pi)^3} \int \exp(-i|x|\sqrt{m^2 + k^2})\, d^3k / \sqrt{k^2 + m^2}$$

By mimicking the analysis of Example 6, we see that $|x|^{2n} f_t^+(x^2; m^2)$ is bounded so long as $n \geq 2$ (Problem 72).

Finally, since $\hat{\Delta}_+$ is real, $\Delta_+(-x) = \overline{\Delta_+(x)}$ proving (f). ∎

Corollary The product $\theta(x_0)\,\Delta_+(x, m^2)$ exists where $\theta(x_0)$ is defined by $\theta(f) = \int_{x_0 \geq 0} f(x)\, d^3x$.

Proof $WF(\theta) = \{\langle 0, \mathbf{x}, \pm\lambda, 0\rangle \,|\, \mathbf{x} \in \mathbb{R}^3, \lambda \in \mathbb{R}_+\}$ so $WF(\theta) \oplus WF(\Delta_+)$ does not contain any vector of the form $\langle x, 0\rangle$. Thus, by Theorem IX.45, the product exists. ∎

NOTES

Section IX.1 J. Fourier's original argument for the inversion formula appears in his classic *La Théorie Analytique de Chaleur*, Didot, Paris, 1822. Although his argument would not be considered a "rigorous proof" by modern standards, it contained the main ideas of the proof we have presented. The approach of first defining the Fourier transform on $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{S}'(\mathbb{R}^n)$ and then restricting to the classical L^p spaces is due to L. Schwartz and is described in *Théorie des Distributions*, Vol. II, Hermann, Paris, 1954. Schwartz's lucid book is the basic reference for the study of the Fourier transform on spaces of distributions and the theory of convolutions of distributions.

The Hermite expansion discussed in the Appendix to Section V.3 can be used to provide short proofs of the Fourier inversion and Plancherel theorems since $\hat{\varphi}_n(k) = (-i)^n \varphi_n(k)$.

Section IX.2 The Riemann–Lebesgue lemma was first proven for a restricted class of functions in B. Riemann, "Ueber der Darstellbarkeit einer Function durch einen trigonometrische Reihe" in *Math. Werke*, Teubner, 1876, pp. 213–253, and for all of L^1 in H. Lebesgue, "Sur les Séries Trigonométriques," *Ann. Sci. Ecole Norm. Sup.* **20** (1903), 453–485. The Plancherel theorem appears in M. Plancherel, "Contribution à l'étude de la représentation d'un fonction arbitraire par des intégrales définies," *Rend. Circ. Mat. Palermo* **30** (1910), 289–335. The Hausdorff–Young theorem was first proven in W. Young: "Sur la généralisation du théorème de Parseval," *C. R. Acad. Sci. Paris Sér. A-B* **155** (1912), 30–33; and extended in F. Hausdorff, "Eine Ausdehnung des Parselvalschen Satzes über Fourierreihen," *Math. Z.* **16** (1923), 163–169.

The original proof of Bochner's theorem appears in S. Bochner, *Vorlesungen über Fouriersche Integrale*, Akademie-Verlag, Berlin, 1932. For a proof of the generalization to distributions, see Schwartz's book. The proof of Bochner's theorem which we give depends on Stone's theorem. Conversely, it is possible to derive Stone's theorem from Bochner's theorem, see E. Hopf: *Ergodentheorie*, Springer-Verlag, Berlin, 1937, or F. Riesz and B. Sz.-Nagy: *Functional Analysis*, Ungar, New York, 1955.

In some sense, the "natural" setting for the L^p theory of the Fourier transform is on an arbitrary locally compact abelian group; see Chapters XIV and XV.

Section IX.3 The close relationship between the support properties of a function and the analyticity properties of its Fourier transform was first developed by R. Paley and N. Wiener in *Fourier Transforms in the Complex Domain*, Amer. Math. Soc. Colloqium Publication, Providence, Rhode Island, 1934. Their work concerned L^2 functions and L^2 boundary values (see below). Nevertheless, a whole class of theorems relating support properties to analyticity properties are usually called Paley–Wiener theorems. The connection between analyticity and the Fourier Transform was further studied by E. C. Titchmarsh, *Introduction to the Theory*

of Fourier Integrals, Oxford Univ. Press (Clarendon), London and New York, 1937. The generalization to distributions with compact support was first proven in L. Schwartz, "Transformation de Laplace des distributions," *Comm. Sém. Math. Lund*, tome suppl. dédié à M. Riesz (1952). A more detailed relation between support and analyticity for functions supported on compact, convex, balanced sets is given in Problem 22.

The idea of regarding the Fourier transforms of more general distributions as the boundary values of analytic functions is also due to Schwartz who proved that if $T \in \mathscr{S}'(\mathbb{R}^n)$ has support in a cone Γ, then $F(\lambda - i\eta t) = \widehat{e^{-t\eta \cdot x}T}$ has polynomial growth in the sense of estimates (i) and (ii) as $t \to \infty$ and as $t \to 0$. To prove this weaker version of one half of Theorem IX.16, one does not need the lemma of Bros–Epstein–Glaser. If $a \in \Gamma$, one chooses a C^∞ function φ so that supp $\varphi \in \Gamma - a$ and $\varphi(x) = 1$ for $x \in \overline{\Gamma}$. Then $F(\lambda - it\eta) = \widehat{e^{-t\eta \cdot x}\varphi(x)T}$ is analytic in $\mathbb{R}^n - i\Gamma^*$, satisfies the growth properties, and has $\hat{T}$ as a boundary value. However, to obtain the estimate (IX.13) which gives polynomial growth near the whole boundary of $\mathbb{R}^n - i\Gamma^*$, one needs the Bros–Epstein–Glaser lemma which was proven in J. Bros, H. Epstein, and V. Glaser, "On the connection between analyticity and Lorentz covariance of Wightman functions," *Comm. Math. Phys.* **6** (1967), 77–100. The proof we give of the second half of Theorem IX.16 is due to L. Gårding (unpublished). His proof is based on the ideas of Köthe and Tillman who realized that a necessary condition for an analytic function to have distribution boundary values on a smooth boundary is polynomial growth; see G. Köthe, "Die Randverteilungen Analytischer Funktionen," *Math. Z.* **57** (1952), 13–33 and H.-G. Tillman, "Randverteilungen analytischer Funktionen und Distributionen," *Math. Z.* **59** (1953), 61–83. We remark that we have stated and proved Theorem IX.16 for a spherically symmetric cone, $\Gamma_{a,\theta}$, but the same proof may be carried through for an arbitrary convex cone (Problem 23). Then Γ^* is given by $\Gamma^* = \{\eta | \eta \cdot x \geq 0 \text{ for all } x \in \Gamma\}$.

There is another formulation of the Paley–Wiener-type theorems in terms of L^2 functions. Suppose $f \in L^2(0, \infty)$. Then $F(\lambda - i\eta) = (2\pi)^{-1/2} \int_0^\infty e^{-i\lambda x} e^{-\eta x} f(x)\, dx$ satisfies

(i) F is an analytic function in the open lower half-plane,

(ii)

$$\sup_{\eta \geq 0} \left\{ \int_{-\infty}^{\infty} |F(\lambda - i\eta)|^2 \, d\lambda \right\} < \infty$$

and

(iii)

$$\int_{-\infty}^{\infty} |F(\lambda - i\eta) - \hat{f}(\lambda)|^2 \, d\lambda \to 0 \qquad \text{as} \quad \eta \to 0$$

by the Lebesgue dominated convergence theorem. That is, $F(\lambda - i\eta)$ takes on the boundary value $\hat{f}(\lambda)$ in the sense of L^2. Analytic functions in the open lower half-plane satisfying (i), (ii), and (iii) are said to belong to the **Hardy–Lebesgue class**, $\mathscr{H}^2(\mathbb{R})$. In the book by Paley and Wiener cited above, the converse statement is proven. Namely, if $F(\lambda - i\eta)$ is in the Hardy–Lebesgue class, then there is a function $f \in L^2(0, \infty)$ so that $F(\lambda - i\eta) = \widehat{e^{-\eta x} f}$ and $F(\lambda - i\eta) \xrightarrow{L^2} \hat{f}(\lambda)$ as $\eta \downarrow 0$. Another related theorem says that $\widehat{e^{-\eta x} f(x)} \in L^2(\mathbb{R})$ for all $\eta \in (\alpha, \beta)$, an open interval containing zero, if and only if $\hat{f}(\lambda)$ has an analytic continuation $\hat{f}(\lambda - i\eta)$ to the strip $\alpha < \eta < \beta$ and $\int_{-\infty}^{\infty} |\hat{f}(\lambda - i\eta)|^2 \, d\lambda < \infty$ for each $\eta \in (\alpha, \beta)$. The reader can easily formulate the generalization of these theorems to several variables.

By Theorem IX.13, if a function f falls off faster than any exponential, then its Fourier transform is an entire function. There are connections between the type of the analytic function

and the detailed rate of falloff; see L. Ehrenpreis, *Fourier Analysis in Several Complex Variables*, Wiley (Interscience), New York, 1970.

Section IX.4 L^p estimates aroused interest very early in the development of functional analysis. Young's inequality was proven in W. Young, "The determination of the summability of a function," *Proc. London Math. Soc.* **12** (1913), 71–78. The Hardy–Littlewood inequality appeared in G. Hardy and J. Littlewood, "Some properties of fractional integrals, I" *Math. Z.* **27** (1928), 565–608. Earlier a similar inequality for sequence spaces appeared in G. Hardy, J. Littlewood, and G. Pólya, "The maximum of a certain bilinear form," *Proc. London Math. Soc.* **25** (1926), 265–268. Their work is essentially a generalization of Hilbert's work on the bilinear form $\sum_{m,n} a_n b_m/(n+m)$, see H. Weyl, *Singulare Integralgleichungen mit besonderer Beruchsichtigung des Fourierschen Integraltheorems*, Inaugural Dissertation, Göttingen, 1908. Sobolev proved his generalization by reducing to the case $n = 1$ in S. Sobolev, "Sur un théorème d'analyse fonctionelle," *Mat. Sb.* (Recueil Math.) **46** (1938), 471–496. The proof was greatly simplified in N. du Plessis, "Some theorems about the Riesz fractional integral," *Trans. Amer. Math. Soc.* **80** (1955), 124–134.

The Hausdorff–Young theorem states: if $p^{-1} + q^{-1} = 1$ and $1 \le p \le 2$, then the norm of the Fourier transform from L^p to L^q is less than or equal to $(2\pi)^{n(1/2-1/p)}$. It has recently been proven in W. Beckner, "Sharp inequalities in Fourier Analysis," *Bull. Amer. Math. Soc.* (to appear) that the norm is actually equal to

$$C(p,q) = \left[\left(\frac{p}{2\pi}\right)^{1/p} \Big/ \left(\frac{q}{2\pi}\right)^{1/q}\right]^{1/2}$$

That the norm could not be smaller than this constant can be seen from the fact that $\|\hat{f}\|_q = C(p,q)\|f\|_p$ if $f = e^{-x^2/2}$.

The Riesz–Thorin theorem was first proven by M. Riesz, "Sur les maxima des formes bilinéaires et sur les fonctionelles linéaires," *Acta Math.* **49** (1926), 465–497. The idea of using complex methods to prove the theorem is due to C. Thorin, "Convexity Theorems," *Comm. Sém. Math. Lund*, **9** (1948). The idea of extending the Riesz–Thorin theorem to analytic families is due to E. Stein, "Interpolation of Linear Operators," *Trans. Amer. Math. Soc.* **83** (1956), 482–492.

Before the weak L^p spaces were formally defined, inequalities were proven which we would now describe as saying that a certain map is bounded from L^p to weak L^p. The weak L^p spaces were then a natural abstraction. The inequalities appeared first in the L^1 context in G. Hardy and J. Littlewood, "A maximal theorem with function theoretic applications," *Acta Math.* **54** (1930), 81–116, and then in the L^p context in the Marcinkiewicz paper quoted below.

The Marcinkiewicz theorem was announced in J. Marcinkiewicz, "Sur l'interpolation d'operateurs," *C. R. Acad. Sci. Paris* **208** (1939), 1272–1273, and was proven in full generality by A. Zygmund, "On a theorem of Marcinkiewicz concerning interpolation of operators," *J. Math.* **35** (1956), 223–248. Hunt's theorem appeared in R. Hunt, "An extension of the Marcinkiewicz theorem to $L(p,q)$ spaces," *Bull. Amer. Math. Soc.* **70** (1964), 803–807.

The $L(p,q)$ spaces are a generalization of the weak L^p spaces and were introduced by G. Lorentz in "On some new functional spaces," *Ann. Math.* **51** (1950), 37–55. Suppose that $\langle M, \mu\rangle$ is a measure space. For each measurable function f on M we can define a measurable function on $\mathbb{R}$ by

$$f^*(x) = \inf\{y > 0 \,|\, \lambda_f(y) \le x\}$$

where $\lambda_f(y) = \mu\{x \mid |f(x)| > y\}$ is the distribution function of f. Now define $L(p, q)$ to be the set of functions on M so that $\|f\|^*_{p,q} < \infty$ where

$$\|f\|^*_{pq} = \begin{cases} \left(\frac{q}{p}\int_0^\infty [t^{1/p} f^*(t)]^q \frac{dt}{t}\right)^{1/q}, & 1 < p < \infty \\ & 1 < q < \infty \\ \sup_{t>0}\{t^{1/p} f^*(t)\}, & 1 < p \le \infty, q = \infty \end{cases}$$

Thus $L^p = L(p, p)$ and $L^p_w = L(p, \infty)$. In fact, it can be shown that if $1 < q_1 \le p \le q_2 \le \infty$, then

$$L(p, q_1) \subset L^p \subset L(p, q_2) \subset L^p_w$$

For a discussion of these spaces and the related interpolation theorems see R. Hunt, "On $L(p, q)$ spaces," *Enseignement Math.* **12** (1966), 247–276. A very readable discussion of interpolation theorems (in particular, a proof of the Marcinkiewicz theorem) may be found in E. Stein and G. Weiss: *Introduction to Fourier Analysis on Euclidean Spaces*, Princeton Univ. Press, Princeton, New Jersey, 1971.

The abstract interpolation theory which we present in the appendix to Section IX.4 is due to A. Calderón, "Intermediate spaces and interpolation, the complex method," *Studia Math.* **24** (1964), 113–190 and J. Lions, "Théorèmes de traces et d'interpolation I, II," *Ann. Scuola Norm. Sup. Pisa* **13** (1959), 389–403; **15** (1960), 317–331; III: *J. Math. Pures Appl.* **42** (1963), 195–203. There are other methods of abstract interpolation. For a description of these and related topics, see the review article by S. Krein and I. Petunin, "Scales of Banach spaces," *Russian Math. Surveys* **21** (1966), 83–157.

The Hadamard three line theorem is just one of a large class of theorems called Phragmén–Lindelöf theorems which are essentially generalizations of the maximum principle to certain unbounded domains. The original papers are E. Phragmén, "Sur une extension d'un théorème classique de la théorie des fonctions," *Acta Math.* **28** (1904), 351–368 and E. Lindelöf and E. Phragmén, "Sur une extension d'un principe classique de l'analyse et sur quelques propriétés des fonctions monogènes dans le voisinage d'un point singulièr," *Acta Math.* **31** (1908), 381–406. In the bounded case, the three line theorem was announced in J. Hadamard, "Sur les fonctions entières," *Bull. Soc. Math. France* **24** (1896), 186–187.

The material discussed in Example 2 of the Appendix is a special case of noncommutative integration theory. In general one would like to define analogues of the L^p spaces for any von Neumann algebra (in our case the algebra is just $\mathscr{L}(\mathscr{H})$). The basic references for this theory are J. Dixmier, "Formes linéaires sur un anneau d'opérateurs," *Bull. Soc. Math. France* **81** (1953), 9–39; I. Segal, "A non-commutative extension of abstract integration," *Ann. Math.* **57** (1953), 401–457, *Correction* **58** (1953), 595–596; and R. Kunze, "$\mathscr{L}_p$ Fourier transforms on locally compact unimodular groups," *Trans. Amer. Math. Soc.* **89** (1958), 519–540. Some of the proofs we use follow the ideas and suggestions of E. Nelson, "Notes on non-commutative integration," *J. Functional Analysis* **15** (1974), 103–116.

Section IX.5 The Malgrange–Ehrenpreis theorem was proven independently by B. Malgrange: "Existence et approximation des solutions des équations aux dérivées partielles et des equations de convolution," *Ann. Inst. Fourier (Grenoble)* **6** (1955–56), 271–355, and L. Ehrenpreis: "Solution of some problems of division," *Amer. J. Math.* **76** (1954), 883–903. The use of fundamental solutions has long been a standard technique in the theory of ordinary differential equations and elliptic boundary-value problems. For an introduction to these methods, see R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Vol. I, p. 351,

Wiley (Interscience), 1953. For a more advanced approach, the reader should consult the four books by Stakgold, Friedmann, Agmon, and Hörmander referred to in the Notes to Section V.4.

The Malgrange-Ehrenpreis theorem shows that the equation $P(D)f = \delta$ has a solution in $\mathscr{D}'(\mathbb{R}^n)$. It is a natural question to ask whether there is a solution that lies in $\mathscr{S}'(\mathbb{R}^n)$. This question was answered in the affirmative by L. Hörmander who proved the stronger statement that $P(D)[\mathscr{S}'] = \mathscr{S}'$ in "On the division of generalized functions by polynomials," *Ark. Mat.* **3** (1958), 555–568. For a general discussion of the ranges of constant coefficient partial differential operators on various spaces of distributions, see M. Agranovich, "Partial differential equations with constant coefficients," *Russian Math. Surveys* **16** (1961), 23–91.

Section IX.6 Weyl's lemma is due to H. Weyl: "The method of orthogonal projection in potential theory," *Duke Math. J.* **1** (1940), 414–444. Sobolev's lemma and spaces were introduced in S. L. Sobolev: "Sur un théorème d'analyse fonctionelle," *Mat. Sb.* **45** (1938), 471–496 and *Certaines applications de l'analyse fonctionelle à la physique mathématique*, Leningrad, 1945.

Weyl's lemma has many generalizations; we will describe two of them. Let Ω be an open bounded set in $\mathbb{R}^n$ and let $C_{\alpha\beta}(x)$, $0 \le |\alpha|, |\beta| \le m$, be a collection of m times continuously differentiable functions. The differentiable operator $A = \sum_{|\alpha|, |\beta| \le m} (-1)^{|\alpha|} D^\alpha C_{\alpha\beta}(x) D^\beta$ is said to be **strongly elliptic** if

$$\operatorname{Re}\left\{ \sum_{|\alpha|, |\beta| = m} C_{\alpha\beta}(x)\xi^\alpha \xi^\beta \right\} \ge C_0 |\xi|^{2m}, \qquad C_0 > 0$$

for all $x \in \Omega$ and all real vectors $\xi \in \mathbb{R}^n$. The following theorem is due to K. O. Friedrichs: "Differentiability of solutions of elliptic partial differential equations," *Math. Scand.* **1** (1953), 55–72.

Theorem Let φ be a weak solution of $A\varphi = f$. If $f \in W_k(\Omega)$, then $\varphi \in W_{k+2m}(\Omega)$.

In "On the theory of general partial differential operators," *Acta Math.* **94** (1955), 161–248, L. Hörmander introduced the following definition. A constant coefficient operator $P(D) = P(i^{-1}\partial/\partial x_1, \ldots, i^{-1}\partial/\partial x_n)$ on Ω (open, not necessarily bounded) is said to be **hypoelliptic** if whenever $f \in C^\infty(\Omega)$, every distribution solution φ of $P(D)\varphi = f$ which is locally L^2 in Ω is in $C^\infty(\Omega)$. Hörmander then proved:

Theorem $P(D)$ is hypoelliptic if and only if for every large constant M_1 there is a positive M_2 so that every zero $\zeta = \xi + i\eta$ of $P(\zeta)$ which satisfies $|\eta| \le M_2$ also satisfies $|\zeta| \le M_1$.

The reader can easily check that Δ is hypoelliptic but $\partial^2/\partial x^2 - \partial^2/\partial t^2$ is not. This theorem has various generalizations to nonconstant coefficient operators, see: L. Hörmander, "On the interior regularity of the solutions of partial differential equations," *Comm. Pure Appl. Math.* **9** (1958), 197–218; B. Malgrange, "Sur une classe d'opérateurs différentielles hypoelliptiques," *Bull. Soc. Math. France* **85** (1957), 283–306; and J. Peetre, "A proof of the hypoellipticity of formally hypoelliptic differential operators," *Comm. Pure Appl. Math.* **16** (1961), 737–747.

Sobolev's lemma (and thus the resulting regularity theorems) can be generalized to various L^p spaces. We say that a function f is in $L^p_k(\mathbb{R}^n)$ if all the partial derivatives of order less than or equal to k are in $L^p(\mathbb{R}^n)$. The generalization of Sobolev's lemma states:

Theorem Suppose that k is a positive integer and $q^{-1} = p^{-1} - k/n$.

(a) If $q < \infty$ (i.e., $p < n/k$), then $L^p_k(\mathbb{R}^n) \subset L^q(\mathbb{R}^n)$ and the natural inclusion map is continuous.

(b) If $q = \infty$ (i.e., $p = n/k$), then the restriction of any $f \in L^p(\mathbb{R}^n)$ to a compact subset of $\mathbb{R}^n$ belongs to $L^r(\mathbb{R}^n)$ for every $r < \infty$.

(c) If $p > n/k$, then every $f \in L^p_k(\mathbb{R}^n)$ can be modified on a set of measure zero so that the resulting function is continuous.

A proof of this theorem and related results may be found in E. Stein, *Singular Integrals and Differentiability Properties of Functions*, Princeton Univ. Press, Princeton, New Jersey, 1970.

The Sobolev inequalities which we have discussed bound an L^q-norm of a function by its L^p-norm and the L^p-norms of some of its derivatives. In some special cases, one can bound the L^q-norm of a function just by the L^p-norms of derivatives if the function is small near infinity. For example, in Section X.13 we will prove and use the estimate

$$\|f\|_6 \leq C \sum_{i=1}^{3} \left\| \frac{\partial f}{\partial x_i} \right\|_2$$

for functions on $\mathbb{R}^3$.

Section IX.7 Most of this section is standard folk wisdom. Theorem IX.31 is due to J. Dollard, "Asymptotic Convergence and the Coulomb Interaction," *J. Math. Phys.* **5** (1964) 729–738.

Section IX.8 The Gårding-Wightman axioms were formulated by L. Gårding and A. S. Wightman in the early 1950's, but they felt it would be premature to publish them until nontrivial examples existed. However, preliminary versions of the axioms appeared in various places, and on the basis of these axioms, the Haag-Ruelle scattering theory was developed (see Section XII.15). This was, in turn, such a beautiful and physical theory that it motivated the publication of the axioms in A. S. Wightman and L. Gårding, "Fields as operator-valued distributions," *Ark. Fys.* **28** (1964), 129–189.

The axioms are thoroughly discussed and many consequences are derived in the two books: *PCT, Spin and Statistics, and All That*, Benjamin, New York, 1964, by R. F. Streater and A. S. Wightman; *The General Theory of Quantized Fields*, Amer. Math. Soc., Providence, Rhode Island, 1965, by R. Jost. These books also contain many references to early work in the subject.

The first question that naturally arises about the Wightman axioms is whether they are consistent. This is not a trivial question since so many mathematical structures are involved. In fact, if the commutator in the local commutativity axiom is changed to an anticommutator, then the axioms are inconsistent (see the spin-statistics theorem below). In Section X.7 we show that the axioms are consistent by showing that, for each m, they are satisfied by the free Klein-Gordon field of mass m. It has not been proven that there are any really interesting field theory models in four space-time dimensions involving interacting particles that satisfy the Wightman axioms. Recently, models obeying the analog of the Wightman axioms in two dimensions have been constructed: see, for example, *Constructive Quantum Field Theory* (G. Velo and A. S. Wightman, eds.), Springer-Verlag, Berlin, 1973, and references therein or B. Simon, *The $P(\varphi)_2$ Euclidean (Quantum) Field Theory*, Princeton University Press, 1974.

Since we still do not possess large classes of mathematical models, let alone a theory, to describe completely the phenomena of elementary particle physics, there has been a great deal of "experimentation" with axioms. This experimentation has consisted of slightly changing the axioms, finding equivalent axiom schemes, or formulating axiom schemes based on some fundamental structures other than the local field structure of the Gårding-Wightman axioms.

If we wish to perturb the axioms slightly, one candidate for change is the purely technical axiom that specifies the test function space be $\mathcal{S}(\mathbb{R}^4)$. In fact, there is a folk theorem that

assures as that a class of formal models known as nonrenormalizable Lagrangian models will lead to Wightman functions which are not polynomially bounded in the tube. This can only be true if a test function space other than $\mathscr{S}(\mathbb{R}^4)$ is used. A whole class of alternative test function spaces which still allow one to phrase the microscopic causality condition are proposed and developed in A. Jaffe, "High energy behavior in quantum field theory, strictly localizable fields," *Phys. Rev.* **158** (1967), 1454-1461.

There are two types of equivalent reformulations of the Wightman axioms. The first is due to Wightman, who wrote down a set of postulates for a sequence of tempered distributions $\{\mathscr{W}_n | \mathscr{W}_n \in \mathscr{S}(\mathbb{R}^{4n})\}$ and proved that the postulates guarantee that the $\mathscr{W}_n$ arise as the Wightman distributions of a unique field theory satisfying the Gårding-Wightman axioms and that conversely the postulates hold in any Wightman field theory. This **reconstruction theorem** appeared in his paper "Quantum field theory in terms of vacuum expectation values," *Phys. Rev.* **101** (1956), 860–866, and is further discussed in Chapter XVII. Wightman's paper did not contain a translation of the axiom of uniqueness of the vacuum to properties of the $\mathscr{W}_n$. This was later added due to work of K. Hepp, R. Jost, D. Ruelle, and O. Steinmann, "Necessary conditions on Wightman functions," *Helv. Phys. Acta* **34** (1961), 542-544, and H. Borchers, "On the structure of the algebra of field observables," *Nuovo Cimento* **24** (1962), 214–236.

A second reformulation of the Wightman axioms is in terms of the **Schwinger functions**, that is the restriction of the Wightman functions to those points in the permuted forward extended tube (i.e., the union of the extended forward tube and its images under permutation of the x-space coordinates) which have purely real spatial coordinates and purely imaginary time coordinates. This reformulation is connected with the Euclidean approach to field theory which we discuss below, so we temporarily defer the historical notes on its development. Axioms on the Schwinger functions equivalent to the Wightman axioms can be found in K. Osterwalder and R. Schrader, "Axioms for Euclidean Green's functions, I," *Comm. Math. Phys.* **31** (1973), 83–112; II, (to appear).

Finally, there are axiom schemes which involve as fundamental structures objects that are distinct from purely local fields. One version emphasizes the role of "asymptotic fields" and thereby makes a direct connection with scattering theory. This is the LSZ axiom scheme of H. Lehmann, K. Symanzik and W. Zimmerman, "Zur Formulierung Quantisierter Feldtheorien," *Nuovo Cimento* **1** (1955), 205–225, "On the formulation of quantum field theories, II," *Nuovo Cimento* **6** (1957), 319–333. As a consequence of the machinery of Haag–Ruelle scattering theory (see Section XII.15), K. Hepp proved that a version of the LSZ axioms holds in any Wightman theory which is supplemented by suitable additional hypotheses on the mass spectrum. See K. Hepp, "On the connection between the LSZ and Wightman quantum field theory," *Comm. Math. Phys.* **1** (1965), 95–111, and his article in *Axiomatic Field Theory* (Brandeis Summer Institute, 1965), Gordon and Breach, New York, 1966.

A second approach to local quantum axiomatics involves the use of Banach algebras. Von Neumann first suggested the use of algebras of bounded operators to axiomatize quantum mechanics and developed much of theory of W^*-algebras ("von Neumann algebras") for this purpose. His work was clarified and expanded by I. Segal in "Postulates for general quantum mechanics," *Ann. Math.* **48** (1947), 930–947. Throughout the fifties Segal championed an algebraic approach to the problems in field theory and in 1964, R. Haag and D. Kastler formulated a set of axioms in "An algebraic approach to quantum field theory," *J. Math. Phys.* **5** (1964), 848–861; see also, H. Araki, "Local quantum theory, I," in *Local Quantum Theory* (R. Jost, ed.), Academic Press, New York, 1969. The relationship between the Haag–Kastler axioms and the Wightman axioms is not direct. *If* the fields in the Wightman

axioms are self-adjoint, then one can form a family of algebras out of their spectral projections, but it is not clear that they satisfy the Haag-Kastler axioms for technical reasons, e.g., the commutation of fields in the Wightman sense might not imply commutation of the spectral projections (see Section VIII.5). Conversely, it is not clear how to reconstruct the fields from the Haag-Kastler local algebras. Nevertheless, the two sets of axioms are closely related and one expects them both to hold in reasonable models. This has been the case in the two-dimensional models constructed so far. We discuss the algebraic approach to field theory in Chapter XIX.

A third approach involves the analytic continuation to imaginary time where the Poincaré group is replaced by the Euclidean group. On the level of perturbation theory, this goes back to F. Dyson, "The *S*-matrix in quantum electrodynamics," *Phys. Rev.* **75** (1949), 1736–1755; and on the level of Wightman functions to Wightman's 1956 paper and the Hall-Wightman paper discussed below. It is at this level of continuation of Wightman functions that the Osterwalder-Schrader axioms operate. But there is a level which is probably more specialized in that it does not follow from only the Wightman axioms, in which one looks for Euclidean *fields*, i.e., operators whose expectation values are the Schwinger functions. Such an approach was first advocated by J. Schwinger, "On the Euclidean structure of relativistic field theory," *Proc. Nat. Acad. Sci. U.S.A.* **44** (1958), 956–965, and T. Nakano, "Quantum field theory in terms of Euclidean parameters," *Progr. Theoret. Phys.* **21** (1959), 241–259. The connection of this formulation with probabilistic ideas, such as the Feynman-Kac formula of Section X.10, and with classical statistical mechanics was first emphasized by K. Symanzik in "Euclidean quantum fields, I, equations for a scalar model," *J. Math. Phys.* **7** (1966), 510–525, and in "Euclidean quantum field theory" in *Local Quantum Theory*, (R. Jost, ed.), Academic Press, New York, 1969. Subsequently, E. Nelson, in "Construction of Quantum Fields from Markoff Fields," *J. Functional Analysis* **12** (1973), 97–112, proposed a set of axioms defining a Euclidean field theory and showed that from any such theory, one could construct a quantum field theory satisfying the Wightman axioms. The converse problem of what must be added to the Wightman axioms to enable one to construct a Euclidean theory obeying all Nelson's axioms has not been definitely solved but a partial solution can be found in B. Simon, "Positivity of the Hamiltonian semigroup and the construction of Euclidean region fields," *Helv. Phys. Acta* **46** (1974), 686–696. This paper includes an example obeying the analogue of the Wightman axioms in one space-time dimension but *not* obeying Nelson's axioms, which shows some additional structure is present in Euclidean field theories.

The Bargmann-Hall-Wightman theorem appeared in D. Hall and A. Wightman, "A theorem on invariant analytic functions with applications to relativistic quantum field theory," *Mat.-Fys. Medd. Danske Vid. Selsk.* **31** (1957), 1–41. V. Bargmann's name is attached to the theorem because of the contributions he made to its proof.

A precursor of the PCT theorem was proven in G. Lüders, "On the equivalence of invariance under time reversal and under particle-antiparticle conjugation for relativistic field theories," *Danske Vid. Selsk. Mat.-Fys. Medd.* **28** (1954), 1–17. The PCT theorem itself was proven in W. Pauli, "Exclusion principle, Lorentz group, and reflection of space-time and charge," in *Niels Bohr and the Development of Physics* (W. Pauli, ed.) Pergamon Press, Oxford, 1955, and R. Jost, "Eine Bemerkung zum CTP Theorem," *Helv. Phys. Acta* **30** (1957), 409–416. For a discussion of the physical significance of the PCT theorem, see S. Gasiorowicz, *Elementary Particle Physics*, Wiley, New York, 1966, pp. 508–519.

The representation of the two-point function given in Theorem IX.34 is called the Källen-Lehmann representation because it was discovered by H. Umezawa and S. Kamefuchi in "The Vacuum in Quantum Electrodynamics," *Progr. Theoret. Phys.* **6** (1951), 543–558. See also G. Källen, "On the definition of the renormalization constants in quantum electro-

dynamics," *Helv. Phys. Acta* **25** (1952), 417–434, and H. Lehmann, "Über Eigenschaften von Ausbreitungsfunktionen und Renormierungskonstanten quantisierter Felder," *Nuovo Cimento* **11** (1954), 342–357.

It is clear from Section IX.8 that the problem of calculating the holomorphy envelopes of the permuted forward tube, the "primitive domain" for the n-point functions is important. For the three-point function, see G. Källen and A. S. Wightman, "The analytic properties of the vacuum expectation values of a product of three scalar local fields," *Mat.-Fys. Skr. Danske Vid. Selsk.* 1 (1958). For a general discussion of analyticity and quantum field theory, see A. S. Wightman, "Quantum field theory and analytic functions of several complex variables," *J. Indian Math. Soc.* **24** (1960), 625–677, or H. Epstein, "Some analyticity properties of the scattering amplitude in quantum field theory," in *Axiomatic Field Theory* (Brandeis Summer Institute, 1965), Gordon and Breach, New York, 1966.

Finally, let us briefly describe the role of "spin" in field theory and the resulting modification of the axioms to accommodate "spinor fields." To explain one of the subtleties associated with spin, we must return to our discussion of dynamics in the notes to Section VIII.11. There, dynamics is described a priori, not by unitary operators, U_t obeying $U_{t+s} = U_t U_s$ but by automorphisms of the states α_t obeying $\alpha_{t+s} = \alpha_t \alpha_s$. It is a theorem that every such automorphism which is a square of some other automorphism is induced by a unitary U unique up to an overall phase transformation $U \to e^{i\theta}U$. Thus U_t can be chosen so that U_t induces α_t and then, by uniqueness up to phase, $U_{t+s} = \lambda(t, s)U_t U_s$ where $\lambda(t, s)$ is a phase factor. In the case of dynamics where the group is $\mathbb{R}$, we can always find $\mu(t)$ with $\lambda(t, s) = \mu(t + s)\mu(t)^{-1}\mu(s)^{-1}$ so that $V(t) = \mu(t)U(t)$ obeys $V(t + s) = V(t)V(s)$. An analysis similar to this works for the Poincaré group but only up to a point. One indeed obtains a strongly continuous map of $\mathscr{L}^\uparrow_+$ into the unitaries obeying $U(AB) = \lambda(A, B)U(A)U(B)$ where $\lambda(A, B)$ is a phase factor. But it is no longer possible, in general, to obtain a strict representation by the substitution $V(A) = \mu(A)U(A)$ for suitable μ. Rather one has the following situation:

There is a group, $SL(2, \mathbb{C})$, and a two-to-one map Λ of $SL(2, \mathbb{C})$ onto $\mathscr{L}^\uparrow_+$. One forms a group $InSL(2, \mathbb{C})$ from $\mathbb{R}^4$ and $SL(2, \mathbb{C})$ by taking $InSL(2, \mathbb{C}) = SL(2, \mathbb{C}) \times \mathbb{R}^4$ in the set equality sense with group operation

$$\langle A, a\rangle\langle B, b\rangle = \langle AB, a + \Lambda(A)b\rangle$$

Thus the map $\tilde{\Lambda}$: $\langle A, a\rangle \to \langle \Lambda(A), a\rangle$ is a two-to-one map of $InSL(2, \mathbb{C})$ to $\mathscr{P}^\uparrow_+$. The basic theorem is that given a map $\tilde{U}$ from $InSL(2, \mathbb{C})$ to the unitaries with $\tilde{U}(AB) = \lambda(A, B) \times \tilde{U}(A)\tilde{U}(B)$, we can find $\mu(\cdot)$ on $InSL(2, \mathbb{C})$ so that $\tilde{V}(A) = \mu(A)\tilde{U}(A)$ obeys $\tilde{V}(AB) = \tilde{V}(A)\tilde{V}(B)$. Given U, a representation up to phase of $\mathscr{P}^\uparrow_+$, we can then define $\tilde{U}$ on $InSL(2, \mathbb{C})$ by $\tilde{U}(A) = U(\tilde{\Lambda}(A))$ and thus associate with U a representation of $InSL(2, \mathbb{C})$. This reduction is due to Bargmann and Wigner in the papers quoted in (4) of our discussion of dynamics in the notes to Section VIII.11; see also Chapter XIV.

Let 1 and -1 be the two elements of $SL(2, \mathbb{C})$ which go into the unit element of $\mathscr{L}^\uparrow_+$ under Λ (in fact, $SL(2, \mathbb{C})$ is the group of all 2×2 complex matrices with determinant 1 and the matrices, 1, -1 go into the unit of $\mathscr{L}^\uparrow_+$ when one defines $\Lambda(A)$ by $\Lambda(A)_{\mu\nu} = \mathrm{tr}(\sigma_\mu A \sigma_\nu A^{-1})$ where $\sigma_0 = 1$ and σ_i are the Pauli matrices). Then an irreducible representation, V, of $InSL(2, \mathbb{C})$ is always one of two types: either $V(-1) = 1$ or $V(-1) = -1$. These types are usually referred to respectively as the integral spin and half-integral spin cases, since in the two cases, the eigenvalues of the angular momentum operator J_z, the infinitesimal generator of the subgroup of $SL(2, \mathbb{C})$ which goes into rotations about the z axis are respectively $0, \pm 1, \pm 2, \ldots$ or $\pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \ldots$. We note that it is natural to extend the analysis of irreducible representations of $InSL(2, \mathbb{C})$ further to a complete set of invariants, namely the mass and the

"spin" (see, e.g., Wigner's paper), but we will only need this $V(-1) = \pm 1$ classification below. We also note that the integral spin cases are precisely those where the representation of $InSL(2, \mathbb{C})$ yields a representation of $\mathscr{P}_+^\uparrow$ rather than just a representation up to a factor.

Next, we define spinor fields, temporarily deferring the discussion of their connection with spin. Let $S(\cdot)$ be a *finite-dimensional* (of necessity not unitary!) irreducible representation of $SL(2, \mathbb{C})$, on a space of dimension d. A **spinor field of type** S is an object obeying the axioms stated for a Hermitian scalar field, with five changes:

(1) The single field $\varphi(\cdot)$ is replaced by a d-tuple of fields $\langle \varphi_1(\cdot), \ldots, \varphi_d(\cdot) \rangle$.
(2) The field $\varphi(f)$, with f real, is not required to be symmetric.
(3) The transformation law, Property 6, is replaced by

$$U(\Lambda, a)\varphi_i(x)U(\Lambda, a)^{-1} = \sum_{j=1}^{d} S(A^{-1})_{ij}\varphi_j(\Lambda x + a)$$

where $\Lambda = \Lambda(A)$.

(4) The vacuum is only required to be cyclic for

$$\{\varphi_1(f), \ldots, \varphi_d(f), \varphi_1^*(f), \ldots, \varphi_d^*(f) \mid f \in \mathscr{S}(\mathbb{R}^4)\}$$

(5) The relation $\varphi(f)\varphi(g) - \varphi(g)\varphi(f) = 0$ if f and g are spacelike separated is replaced by either:

(a) (Böse statistics)

$$\varphi_i(f)\varphi_j(g) - \varphi_j(g)\varphi_i(f) = 0$$
$$\varphi_i^*(f)\varphi_j(g) - \varphi_j(g)\varphi_i^*(f) = 0$$

or

(b) (Fermi statistics)

$$\varphi_i(f)\varphi_j(g) + \varphi_j(g)\varphi_i(f) = 0$$
$$\varphi_i^*(f)\varphi_j(g) + \varphi_j(g)\varphi_i^*(f) = 0$$

Depending on whether $S(-1) = 1$ or $S(-1) = -1$, we refer to integral or half-integral spin spinor fields. One has the remarkable

Theorem (spin and statistics theorem) Let $\{\varphi\}$ be a field of type S. Then, if φ obeys Bose statistics, S has integral spin, and if φ obeys Fermi statistics, S has half-integral spin.

The spin and statistics theorem for free fields appeared in M. Fierz, "Über die relativistische Theorie kräftfreirer Teilchen mit beliebigem Spin," *Helv. Phys. Acta* **12** (1939), 3–37, and W. Pauli, "On the connection between spin and statistics," *Phys. Rev.* **58** (1940), 716–722. For the general case, see G. Lüders and B. Zumino, "Connection between spin and statistics," *Phys. Rev.* **110** (1958), 1450–1453, and N. Burgoyne, "On the connection of spin with statistics," *Nuovo Cimento* **8** (1958), 607–609. When one has a theory with several different fields the relation of the spins to the commutation relations is somewhat complicated; see the Streater-Wightman book and G. F. Dell'antonio, "On the connection of spin with statistics," *Ann. Phys.* **16** (1961), 153–157.

There is also a PCT theorem for spinor fields. The PCT operator Θ acts on the fields by

$$\Theta\varphi_i(x)\Theta^{-1} = \sum_{j=1}^{d} A_{ij}\varphi_j^*(-x)$$

where A is an explicit matrix depending only on S. For a discussion, see the PCT papers quoted above or the Streater–Wightman book.

There has also been some discussion of "infinite spin fields," i.e., fields where $S(A)$ is replaced by some *infinite* dimensional representation of $SL(2, \mathbb{C})$. One difficulty with such fields is that the Bargmann–Hall–Wightman and PCT theorems may fail for them. See A. Oksak and I. Todorov, "Invalidity of the TCP-theorem for infinite-component fields," *Comm. Math. Phys.* **11** (1968), 125–130.

Finally, let us say a word about the connection between spinor fields and the spin of particles. "Particles" enter field theory as eigenstates of the "mass" operator $M = \sqrt{H^2 - \mathbf{P}^2} \equiv (\tilde{P} \cdot P)^{1/2}$. The subspace $\mathscr{H}_m = \{\psi \mid M\psi = m\}$ is left invariant by $InSL(2, \mathbb{C})$ and the representation of $InSL(2, \mathbb{C})$ on $\mathscr{H}_m$ is a direct sum of irreducibles. If there is a single irreducible summand, we say there is only one particle of mass m and its spin is the invariant associated to the representation. In general, there is only a tenuous connection between the "spin" in the S describing the spinor field and the spin of the particles of a theory. However, one critical connection remains: If $\varphi_1, \ldots, \varphi_k$ are fields (not necessarily in the same multiplets and not necessarily distinct), then $\varphi_1(f_1) \cdots \varphi_n(f_n)\psi_0$ can "couple" to one particle states (i.e., is not orthogonal) of half-integral spin (respectively, integral spin) only if an odd number of φ_i's (respectively, even number) are half integral spin. This allows one to relate the physical spin of a particle to its statistics. Other than this one connection, one can say almost nothing, for there can be more particles than fields, or more fields than particles or particles whose spins are unrelated to the spins of the fields (all these phenomena occur with suitably modified free fields based on the simple model of Section X.7).

Section IX.9 The ideas and proof in this section go back to the work of E. Gagliardo, "Caratterizzazioni delle trace sulla frontiera relative ad alcune classi di funzioni in n variabli," *Rend. Sem. Mat. Univ. Padova* **27** (1957), 284–305, and N. Aronszajn and K. Smith, "Theory of Bessel Potentials, I," *Ann. Inst. Fourier (Grenoble)* **11** (1961), 385–475. For a more detailed discussion of the restriction problem, see E. Stein, *Singular Integrals and Differentiability Properties of Functions*, Princeton Univ. Press, Princeton, New Jersey, 1970, Chapter VI.

The restriction results we discuss hold for flat or curved submanifolds. Much more subtle are a class of results which only hold for curved submanifolds. For example, if $f \in L^p(\mathbb{R}^2)$ with $p < \frac{4}{3}$, then $\hat{f}$ may be restricted to an L^2 function on the unit circle (but, if $p > 1$, it may not be possible to restrict it to a piece of coordinate axis). This result and the extensions appear in C. Fefferman, "Inequalities for Strongly Singular Convolution Operators," *Acta Math.* **124** (1970), 9–36.

The geometric measure which we referred to immediately before Theorem IX.39 is a generalization of arc length measure for curves. Intuitively, it is described as follows: At any point $x \in M$, choose an orthonormal set of tangent vectors to M at x and take the Lebesgue measure on the tangent space with respect to these coordinates. Then the measure of a very small set about x is approximately the Lebesgue measure of its normal projection onto the tangent space. In the usual differential geometric language, this is the measure on M associated with the metric on M induced by the natural metric on $\mathbb{R}^n$.

Section IX.10 The elaborate machinery of wave front sets and oscillatory integrals was developed in order to study partial differential operators and not merely for the modest problem of defining products of distributions. We have presented our discussion as an introduction to this machinery. Our treatment is closely patterned on parts of L. Hörmander, "Fourier integral operators, I" *Acta Math.* **127** (1971), 79–183. This paper introduced the notion of wave front set and originally defined it by using pseudo-differential operators (see below). It is a

proposition in Hörmander's paper that his definition is equivalent to the one we use. Notions similar to wave front set can be found in M. Sato, "Hyper-functions and partial differential equations," *Conference on Functional Analysis and Related Topics*, Swets and Zeitlinger, Tokyo, 1969, pp. 91–94. Detailed applications of wave front sets and oscillatory integrals to partial differential equations can be found in J. Duistermaat and L. Hörmander, "Fourier integral operators, II," *Acta Math.* **128** (1972), 183–269.

Fourier integral operators are the natural outgrowth of several lines of development. Pseudo-differential operators arise naturally as a generalization of partial differential operators with nonconstant coefficients. Let $a_i \in C^\infty(\Omega)$, $\Omega \subset \mathbb{R}^n$ and let p_i be a homogeneous polynomial of degree i. Then, for all $\varphi \in C_0^\infty(\Omega)$

$$\sum_{i=1}^{N} a_i(x)p_i(-iD)\varphi(x) = \sum_{i=1}^{N} a_i(x)\widehat{(p_i(\theta)\hat{\varphi}(\theta))}$$

$$= (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{ix\cdot\theta} \left(\sum_{i=1}^{N} a_i(x)p_i(\theta) \right) \hat{\varphi}(\theta)\, d\theta$$

Since p_i is a polynomial of degree i, $\sum_{i=1}^{N} a_i(x)p_i(\theta)$ is a symbol of order N. If we replace $\sum_{i=1}^{N} a_i(x)p_i(\theta)$ by an arbitrary symbol of order N, the corresponding operator

$$(A\varphi)(x) = \int_{\mathbb{R}^n} e^{ix\cdot\theta} a(x, \theta)\hat{\varphi}(\theta)\, d\theta$$

is called a **pseudo-differential operator** of order N. A systematic calculus for such operators was developed in J. Kohn and L. Nirenberg, "On the algebra of pseudo-differential operators," *Comm. Pure Appl. Math.* **18** (1965), 269–305.

Pseudo-differential operators of order zero are called **singular integral operators**. Such operators arose in the classical technique of reducing a boundary value problem for an elliptic operator in a region Ω to an integral equation problem on $\partial\Omega$ (see the example in Section VI.5). For a discussion of these techniques see, for example, L. Hormander, "Pseudo-differential operators and non-elliptic boundary value problems," *Ann. Math.* **83** (1966), 129–209, or R. Seeley, "Elliptic singular integral equations," in *Singular Integrals, Proc. Symp. Pure Math.*, Amer. Math. Soc., Providence, Rhode Island, 1967, 308–315, where a detailed historical review is given.

For nonelliptic equations, it is quite natural to replace $x \cdot \theta$ by a more general phase function and such a procedure was followed by a variety of authors before Hörmander's systematic developments: P. D. Lax, "Asymptotic solutions of oscillatory initial value problems," *Duke J. Math.* **24** (1957), 627–646; D. Ludwig, "Exact and asymptotic solutions of the Cauchy problem," *Comm. Pure Appl. Math.* **13** (1960), 473–508; V. P. Maslov, *Theory of Perturbations and Asymptotic Methods*, Moskov. Gos. Univ., Moscow, 1965 (in Russian; French translation by J. Lascoux and R. Senor published by Dunod, Paris, 1972); G. I. Eskin, "The Cauchy problem for hyperbolic systems in convolutions," *Mat. Sb.* **74** (1967), 262–297; Yu. V. Egorov, "On canonical transformations of pseudo-differential operators," *Usp. Mat. Nauk.* **25** (1969), 235–236; and L. Nirenberg and F. Trèves, "On local solvability of linear partial differential equations, Parts I, II, *Comm. Pure Appl. Math.* **23** (1970), 1–38; 459–510. In particular, Maslov's book contains ideas which have been crucial in further developments.

Wave front sets are especially useful in discussing regularity (and nonregularity) of solutions of partial differential equations. For example, one has the following generalization of the elliptic regularity theorem (see, e.g., Fourier integral operators, II):

Theorem Let $P(x, D) = \sum_{|\alpha| \leq n} a_\alpha(x) D^\alpha$ be a partial differential operator with C^∞ coefficients and let f be a C^∞ function. If $T \in \mathscr{D}'_{\mathbb{R}^n}$ solves $P(x, D)T = f$, then

$$WF(T) \subset \left\{ \langle x, k \rangle \;\middle|\; \tilde{P}(x, k) \equiv \sum_{|\alpha| = n} a_\alpha(x) k^\alpha = 0 \right\} \tag{IX.66}$$

There is a further refinement of this theorem which asserts that if a point (x_0, k_0) in the set on the right-hand side of (IX.66) lies in $WF(T)$, then automatically an entire associated set (the bicharacteristic strip with initial point (x_0, k_0)) lies in $WF(T)$. This refined theory goes under the name "propagation of singularities" and has its roots in geometrical optics.

Example 1 was shown to us by O. E. Lanford, III.

Theorem IX.44f has a natural translation if we consider distributions on a manifold M. It asserts that $WF(T)$ is a subset of the cotangent bundle of M.

Theorem IX.46 has an application to the problem of restricting a distribution to an embedded submanifold, a problem which we discussed from a different point of view in Section IX.9. Let us consider the case of an embedded curve in $\mathbb{R}^n$; for the general case, see Hörmander's paper: "Fourier integral operators, I," Theorem 2.5.11. Let $F: \mathbb{R} \to \mathbb{R}^n$ be an injective C^∞ function obeying: (i) grad $F(t) \neq 0$ for any t; (ii) $\lim_{t \to \pm\infty} |F(t)| = \infty$ (F is called a regularly embedded, proper, simple, smooth curve). Any function $g \in C_0^\infty(\mathbb{R}^n)$ has a "restriction" to the curve F, to wit $F_*(g)(t) = g(F(t))$. Now let $T \in \mathscr{D}'(\mathbb{R}^n)$. Can we find a natural meaning to $F_*(T)$, at least for some set of $T \in \mathscr{D}'(\mathbb{R}^n)$? To do this, we rephrase the definition of $F_*(g)$. Given $f \in C_0^\infty(\mathbb{R})$, let $f\delta_F$ be the distribution in $\mathscr{D}(\mathbb{R}^n)$ given by

$$(f\delta_F)(g) = \int_{-\infty}^{\infty} f(t) g(F(t))\, dt$$

If we think of $F_*(g)$ as a distribution, then

$$F_*(g)(f) = (f\delta_F)(g)$$

More to the point, if we pick a function $\chi \in C_0^\infty(\mathbb{R}^n)$ identically one in a neighborhood of $\{F(t) | t \in \operatorname{supp} f\}$, then

$$F_*(g)(f) = [g(f\delta_F)](\chi) \tag{IX.67}$$

where $g(f\delta_F)$ denotes the product of g and the distribution $f\delta_F$. If $WF(T) \oplus WF(f\delta_F)$ is disjoint from $\{\langle x, 0 \rangle\}$, then we can use (IX.67) to define $F_*(T)$! Thus, we must find $WF(f\delta_F)$. A simple argument (Problem 67) shows that $WF(\delta_F) = \{\langle x, k \rangle | x = F(t); k \cdot \text{grad } F = 0, k \neq 0\}$, the **normal bundle** $N(F)$ to the curve F and that $WF(f\delta_F) \subset WF(\delta_F)$. Thus, by Theorem IX.46, we have:

Theorem If $T \in \mathscr{D}'(\mathbb{R}^n)$ has its wave front set disjoint from the normal bundle $N(F)$, then $F_*(T)$ can be defined by (IX.67) and moreover

$$WF(F_*(T)) \subset F^*(WF(T)) \equiv \{\langle t, \text{grad } F \cdot k \rangle \mid \langle F(t), k \rangle \in WF(T)\}$$

PROBLEMS

1. Find the Fourier transform of $3x^2 + 1$.

†2. Give the details of the convergence of the Riemann sum to the integral at the end of the proof of Theorem IX.1.

3. (a) Let R be a rotation and R^t its transpose. Let $f \in \mathscr{S}$. Prove that $\widehat{f \circ R} = \hat{f} \circ R^t$.
   (b) Let D_λ be the map $D_\lambda x = \lambda x$ on $\mathbb{R}^n$. Let $f \in \mathscr{S}(\mathbb{R}^n)$. Prove that

$$\widehat{f \circ D_\lambda} = \lambda^{-n} \hat{f} \circ D_{\lambda^{-1}}$$

   (c) Let $T \in \mathscr{S}'(\mathbb{R}^n)$. Prove that

$$\widehat{(T \circ R)} = \hat{T} \circ R^t, \qquad \widehat{T \circ D_\lambda} = \lambda^{-n} \hat{T} \circ D_{\lambda^{-1}}$$

4. Compute the Fourier transform of $\mathscr{P}(1/x)$, the Cauchy principle part, by using Equation (V.4).

5. Compute the Fourier transform of $f(x) = e^{-\alpha x^2/2}$ as follows:
   (a) Prove that $-\lambda \hat{f}(\lambda) = \alpha \, d\hat{f}(\lambda)/d\lambda$ and conclude that $\hat{f}(\lambda) = ce^{-\lambda^2/2\alpha}$
   (b) Use the Plancherel theorem to prove $c = 1/\sqrt{\alpha}$.
   (c) Check the Fourier inversion formula explicitly in this example.

6. Let $\mathscr{H} = L^2(\mathbb{R}, e^{-x^2}\,dx)$ and define $\psi_n = x^n \in \mathscr{H}$ for $n = 0, 1, \ldots$.
   (a) Prove that $\sum_{m=0}^{M} ((ik)^m/m!)\psi_m \xrightarrow[M \to \infty]{} e^{ikx}$ in the norm topology on $\mathscr{H}$.
   (b) Suppose $\eta \in \mathscr{H}$ and $(x^m, \eta) = 0$ for all m. Prove $\varphi = 0$. (*Hint*: show that $\eta e^{-x^2} = 0$.)
   (b') Reach the conclusion of (b) without recourse to the Fourier transform. (*Hint*: Use the fact that the functions $(x \pm i)^{-n}$ are total in $C_\infty(\mathbb{R})$ and the formula $(x + i)^{-1} = i \int_0^\infty e^{-s} e^{isx}\,ds$).
   (c) Let $\{H_n\}$ be the orthonormal set obtained from $\{\psi_n\}$ by Gram–Schmidt orthogonalization. Prove that $\{H_n\}$ is a basis for $\mathscr{H}$.
   (d) Prove that $\{H_n(x)e^{-x^2/2}\}_{n=0}^\infty$ is an orthonormal basis for $L^2(\mathbb{R}, dx)$.
   (e) Prove that $H_n(x)e^{-x^2/2}$ is just the nth Hermite function (defined in the Appendix to Section V.3).

7. Let $\{A_n(\lambda)\}$ be the polynomials determined by the formula

$$\sum_{n=0}^{\infty} A_n(\lambda) \frac{\alpha^n}{n!} = e^{-\alpha^2 + 2\alpha\lambda}$$

   Define $\phi_n(\lambda) = (2^n n!)^{-1/2} A_n(\lambda) e^{-\lambda^2/2}$.
   (a) Prove that

$$\phi_n(\lambda) = \frac{(-1)^n}{\sqrt{2^n n!}} e^{\lambda^2/2} \left(\frac{d}{d\lambda}\right)^n e^{-\lambda^2}$$

   so that the $\phi_n(\lambda)$ are just the Hermite functions of the Appendix to Section V.3.
   (b) If $f \in L^2(\mathbb{R}, dx)$ and $(f, \phi_n) = 0$ for all $n = 0, 1, \ldots$, prove that for all a,

$$\int f(x) e^{-(x-a)^2/2}\,dx = 0$$

   (c) Use the Fourier transform to show that if $\int_{\mathbb{R}} f(x)e^{-(x-a)^2/2}\,dx = 0$ for all a, then $f = 0$.
   (d) Conclude that $\{\phi_n\}$ is a basis for $L^2(\mathbb{R}, dx)$.

8. The purpose of this problem is to prove the Plancherel theorem and the inversion formula by using the Hermite functions. Let

$$A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right) \quad \text{and} \quad A^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)$$

(a) If $f \in \mathscr{S}(\mathbb{R}^n)$ prove $\widehat{A^\dagger f}(\lambda) = -i(A^\dagger \hat{f})(\lambda)$.
(b) Prove that $\hat{\phi}_n = (-i)^n \phi_n$.
(c) Supposing the fact that the Hermite functions are a basis for $L^2(\mathbb{R})$, prove the Plancherel theorem and the inversion formula.

9. Suppose that C is a continuous map of $\mathscr{S}(\mathbb{R}^n)$ into $C^\infty(\mathbb{R}^n)$ which commutes with translations. Prove that there is a $T \in \mathscr{S}'(\mathbb{R}^n)$ so that $C(\varphi) = T * \varphi$, for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$. (*Hint*: If $T \in \mathscr{S}'(\mathbb{R}^n)$ and $\varphi \in \mathscr{S}(\mathbb{R}^n)$, then $T(\varphi) = (T * \tilde{\varphi})(0)$.)

10. Prove directly (without using the Fourier transform) that for fixed $f \in \mathscr{S}(\mathbb{R}^n)$, the map $g \mapsto f * g$ is a continuous linear transformation of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$.

11. Let μ_1 and μ_2 be finite Borel measures on $\mathbb{R}^n$ and define

$$(\mu_1 * \mu_2)(E) = \int_{\mathbb{R}^n} \mu_1(E - y)\, d\mu_2(y)$$

(a) Prove that $\mu_1 * \mu_2$ is a finite Borel measure on $\mathbb{R}^n$, that $\mu_1 * \mu_2 = \mu_2 * \mu_1$, and that for any $f \in C_\infty(\mathbb{R}^n)$

$$(\mu_1 * \mu_2)(f) = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(x + y)\, d\mu_1(x)\, d\mu_2(y)$$

(b) Prove that $\mu_1 * \mu_2$ is absolutely continuous with respect to Lebesgue measure if either μ_1 or μ_2 is absolutely continuous with respect to Lebesgue measure. Give an example where $\mu_1 * \mu_2$ is not absolutely continuous.

12. The Fourier transforms of Borel measures of mass one on $\mathbb{R}^n$ are sometimes called "characteristic functions." A characteristic function $E(\lambda)$ is said to be **infinitely divisible** if for all positive integers n, there exists a characteristic function $E_n(\lambda)$ so that $E(\lambda) = (E_n(\lambda))^n$.
(a) Let μ be a Borel measure of mass one on $\mathbb{R}$ and let E be the corresponding characteristic function. Prove that E is infinitely divisible if and only if for all n there is a Borel measure of mass one, μ_n, so that

$$\mu = \underbrace{\mu_n * \mu_n * \cdots * \mu_n}_{n \text{ times}}$$

(b) Show that

$$E(\lambda) = \exp(i\alpha\lambda - \tfrac{1}{2}\beta\lambda^2) + \int_{-\infty}^{\infty} (e^{i\lambda x} - 1)\, d\rho$$

is an infinitely divisible characteristic function if $\alpha \in \mathbb{R}$, $\beta \geq 0$, and ρ is a Borel measure of finite mass on $\mathbb{R}$. Give a (convolution) formula for the corresponding measure in terms of α, β, and ρ. What is the corresponding measure if $\rho = 0$? What is the corresponding measure if $\alpha = 0 = \beta$ and $\rho = \delta(x - x_0)$?

Remark: There is a characterization of the Fourier transforms of all infinitely divisible distributions known as the Lévy-Khinchin formula. See, for example, L. Breiman, *Probability*, Addison Wesley, Reading, Massachusetts, 1968, 193–195.

13. Let Ω be an open set in $\mathbb{R}^n$, K a compact subset of Ω. Prove that there is a function in $C_0^\infty(\Omega)$ which is equal to one on K. (*Hint*: See Problem 61 of Chapter V.)

14. The purpose of this exercise is to prove the Fourier inversion formula by an alternative method. Suppose that $f \in \mathscr{S}(\mathbb{R}^n)$.
(a) Prove that $\lim_{\varepsilon \downarrow 0} \int_\varepsilon^{1/\varepsilon} ((\sin x)/x)\, dx$ exists. Call it d. Now, show that

$$\lim_{\varepsilon \downarrow 0} \int_\varepsilon^{1/\varepsilon} \frac{\sin Rx}{x}\, dx = d \qquad \text{for any } R > 0$$

(*Hint*: Use facts about telescoping series.)
(b) Prove that

$$\int_0^\infty \left[\frac{f(y-u) + f(y+u)}{2} - f(y) \right] \frac{\sin Ru}{u}\, du \xrightarrow[R \to \infty]{} 0$$

(Use the Riemann-Lebesgue lemma.)
(c) Using (b) conclude that

$$4df(y) = \lim_{R \to \infty} \int_{-\infty}^{\infty} \left(\int_{-R}^{R} e^{i(y-x)\cdot k} f(k)\, dk \right) dx$$

(d) Prove that $f(y) = (\sqrt{2\pi}/4d) \int_{-\infty}^{\infty} e^{iky} \hat{f}(y)\, dk$.
(e) By letting $f(x) = e^{-x^2/2}$, conclude that $d = \pi/2$.

15. The purpose of this exercise is to provide an alternative proof of the Plancherel theorem.
(a) Prove directly that if $f, g \in \mathscr{S}(\mathbb{R}^n)$

$$\widehat{f * g} = (2\pi)^{n/2} \hat{f} \hat{g}$$

(b) Letting $\tilde{f}(x) = f(-x)$, prove that

$$(f * \tilde{f})(y) = \int |\hat{f}(k)|^2 e^{iky}\, dk$$

(c) Set $y = 0$ and conclude that

$$\int |f(x)|^2\, dx = \int |\hat{f}(k)|^2\, dk$$

16. Prove that the map $L^1(\mathbb{R}^n) \xrightarrow{\wedge} C_\infty(\mathbb{R}^n)$ is not onto by exhibiting a function in $C_\infty(\mathbb{R}^n)$ which is not in its range.

17. The purpose of this problem is to develop the Fourier transform on $L^1(\mathbb{R}^n)$ without reference to $\mathscr{S}(\mathbb{R}^n)$.
(a) If $f \in L^1(\mathbb{R}^n)$, prove directly that

$$\hat{f}(\lambda) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i\lambda x} f(x)\, dx$$

is a bounded continuous function. (*Hint*: Use the dominated convergence theorem.)

(b) If $f \in L^1(\mathbb{R}^n)$, prove that $\hat{f}(\lambda) \to 0$ as $|\lambda| \to \infty$. (*Hint*: Prove that $2\hat{f}(\lambda) = (2\pi)^{-n/2} \int e^{-ix\lambda}(f(x) - f(x - \pi\lambda/|\lambda|^2)\, dx$.

(c) Prove directly that $(2\pi)^{n/2}\widehat{fg} = \hat{f} * \hat{g}$.

18. Find a function $f(x)$ that satisfies all the conditions in the definition of "functions of positive type" except continuity. To which function of positive type is $f(x)$ equal a.e.?

19. Display a distribution of positive type that is not a function. What is its Fourier transform?

*20. Prove the Bochner-Schwartz theorem (Theorem IX.10). (*Hint*: Mimic our proof of Bochner's theorem using the inner product $(\varphi, \psi) = T(\tilde{\bar{\varphi}} * \psi)$ and the formula $T(\tilde{\bar{\varphi}} * \varphi_x) = (T * \bar{\varphi} * \tilde{\varphi})(x)$.)

21. What does the generalization of the Paley-Wiener theorem to distributions with compact support say about the Fourier transform of distributions with support at the origin? Compute the same result directly by using Theorem V.11.

22. Let C be a convex, compact, balanced set in $\mathbb{R}^n$. Let

$$C^\circ = \{k \mid k \cdot x \geq -1 \text{ for all } x \in C\}$$

be its polar. Let ρ be the Minkowski functional of C°, i.e.,

$$\rho(\eta) = \sup_{x \in C}(\eta \cdot x) = \inf_{\lambda > 0}\{\lambda \mid \lambda \in \mathbb{R},\ \lambda\eta \in C^\circ\}$$

Prove the following version of the Paley-Wiener theorem:

A function $f \in \mathscr{S}(\mathbb{R}^n)$ has support in C if and only if $\hat{f}$ is the restriction to $\mathbb{R}^n$ of an entire function $\hat{f}(z)$ which obeys the condition that for any n there is a constant D_n so that

$$|\hat{f}(z)| \leq D_n(1 + |z|^2)^{-n} e^{-\rho(\operatorname{Im} z)}$$

23. Prove the extension of Theorem IX.16 in the case where $\Gamma_{a,\theta}$ is replaced with an arbitrary proper, open, convex cone Γ and

$$\Gamma^* = \{\eta \mid \eta \cdot x \geq 0 \text{ for all } x \in \Gamma\}$$

24. (a) Let f be a measurable function on a measure space $\langle M, \mu\rangle$. Let

$$m_f(t) = \mu\{x \mid |f(x)| > t\}$$

Prove that if $f \in L^p(M, d\mu)$, then

$$\int_M |f|^p\, d\mu = -\int_0^\infty t^p\, dm_f(t) \qquad \text{(Stieltjes integral)}$$

(b) Prove that if $f \in L^p(M, d\mu)$, then

$$m_f(t) \leq \|f\|_p^p t^{-p}$$

(c) Prove that $f \in L^p(M, d\mu)$ if and only if

$$\int_0^\infty t^{p-1} m_f(t)\, dt < \infty$$

and in that case $\|f\|_p^p = p\int_0^\infty t^{p-1} m_f(t)\, dt$.

25. Prove that if $r < p < s$ and $f \in L^r_w \cap L^s_w$, then $f \in L^p$ and

$$\|f\|_p^p \le \left(\frac{1}{p-r} + \frac{1}{s-p}\right)[\|f\|_{r,w}^r]^{(s-p)/(s-r)}[\|f\|_{s,w}^s]^{(p-r)/(s-r)}$$

26. (Hunt's interpolation theorem)
   (a) Let $1 \le p_0 < p_1 < \infty$, $0 < t < 1$, $p^{-1} = tp_1^{-1} + (1-t)p_0^{-1}$. Show that $f \in L^p_w$ if and only if there exists a C so that for $\lambda > 0$, f can be decomposed as $f = f_{0,\lambda} + f_{1,\lambda}$ with $f_{0,\lambda} \in L^{p_0}$, $f_{1,\lambda} \in L^{p_1}$ and

$$\|f_{0,\lambda}\|_{p_0} \le C|\lambda|^{1-(p/p_0)}, \qquad \|f_{1,\lambda}\|_{p_1} \le C|\lambda|^{1-(p/p_1)}$$

   (*Hint*: Try $f_{0,\lambda}(x) = f(x)$ if $|f(x)| > \lambda$.)
   (b) Prove that $\|f\|_{p,w} = C$, where C is the smallest constant which can be used in part (a).
   (c) Use (a) and (b) to prove Hunt's interpolation theorem.

27. (a) Let $f \in L^p(M, d\mu)$. Prove that $t^p\mu\{x \mid |f(x)| > t\} \to 0$ as $t \to 0$ or ∞.
   (b) Put a metric on $L^p_w(M, d\mu)$ by $\rho(f, g) = \|f - g\|_{p,w}$. Prove that $L^p(\mathbb{R}^n, dx)$ is not dense in $L^p_w(\mathbb{R}^n, dx)$ in this metric.

   Note: In Hunt's theorem, T is defined on L^p_w not by a density argument (which does not work by the above) but by showing that if $f \in L^p_w$ for $p_0 < p < p_1$, then f can be written $f = f_0 + f_1$ with $f_0 \in L^{p_0}$ and $f_1 \in L^{p_1}$. Thus we can define $Tf = Tf_0 + Tf_1$.

†28. Fill in the details in the derivation of Sobolev's inequality (Example 3, Section 4).

29. Prove that the extension of the Fourier transform to $L^p(\mathbb{R}^n)$ given by the Hausdorff-Young theorem coincides with the restriction to $L^p(\mathbb{R}^n)$ of the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$.

30. (weak Hausdorff-Young) Prove that $\hat{f} \in L^q_w$ if $f \in L^p_w$ where $1 < p < 2$ and $p^{-1} + q^{-1} = 1$.

31. Prove Young's Theorem in the case $1 \le p, q \le 2$, $r \ge 2$ by using Hölder's inequality and the Hausdorff-Young theorem twice.

32. (weak Young theorem) Use the generalized Young inequality to prove that $f * g \in L^r_w$ if $f \in L^p_w$, $g \in L^q_w$ and $p^{-1} + q^{-1} = 1 + r^{-1}$, $1 < p, q, r < \infty$.

*33. Provide a proof of Proposition 1 of the Appendix to Section IX.4 which does not use interpolation.

34. (a) Let $\|\cdot\|_0$ be the L^2 norm on $C_0^\infty(\mathbb{R}^n)$ and let $\|f\|_1 = \|f\|_0 + |f(0)|$. Show that $\|\cdot\|_0$ and $\|\cdot\|_1$ are not consistent. Compute the interpolation spaces X_t anyway.
   (b) Let $X = C[0, 1]$. Define $\|f\|_0 = \int_0^1 |f(x)|\,dx$ and let $\|f\|_1 = \sum_{n=1}^\infty 2^{-n}|f(r_n)|$ where $\{r_n\}_{n=1}^\infty$ is an ordering of the rationals. Show that $\|f\|_+ = 0$ for all $f \in X$.

†35. Fill in the details of the proof that $X_t = \mathscr{H}_{m_t}$ in Example 3 of the Appendix to Section IX.4.

36. Suppose $\alpha \in \mathbb{R}$ and $p > 1$. Define H^p_α to be the completion of $C_0^\infty(\mathbb{R}^n)$ in the norm $\|\varphi\|_{\alpha,p} = \|((1 + k^2)^{\alpha/2}\hat{\varphi}\|_p$.
   (a) Show that the norms $\|\cdot\|_{\alpha,p}$ are consistent.
   (b) Let $p_0, p_1 > 1$ and $\alpha_0, \alpha_1 \in \mathbb{R}$ be fixed. Prove that the interpolating spaces X_t between $H^{p_0}_{\alpha_0}$ and $H^{p_1}_{\alpha_1}$ are equal to $H^{p_t}_{\alpha_t}$ for each $0 \le t \le 1$ where $p_t = tp_1^{-1} + (1-t)p_0^{-1}$ and $\alpha_t = t\alpha_1 + (1-t)\alpha_0$.

*37. Let X be a complex vector space with consistent norms $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$. The purpose of this problem is to sketch the proof of the statement $X_t = \tilde{X}_t$ in the Appendix to Section 4. We use the notation introduced there.

(a) Show that if $x \in X_0 \cap X_1$, there exists $x_n \in X$ so that $x_n \to x$ in both the $\|\cdot\|^{(0)}$-norm and the $\|\cdot\|^{(1)}$-norm.

(b) Use (a) and the inequality

$$\|x\|_+ \leq \|x\|^{(t)} \leq \max\{\|x\|^{(0)}, \|x\|^{(1)}\}$$

to prove that it is sufficient to prove that $X_0 \cap X_1$ is dense in $\tilde{X}_t$ in order to conclude that $\tilde{X}_t = X_t$.

(c) Define $\mathscr{F}_\infty$ to be those $f \in \mathscr{F}$ such that

(i) $\|f(ia)\|^{(0)} \to 0$ as $a \to \pm\infty$

(ii) $\|f(1 + ia)\|^{(1)} \to 0$ as $a \to \pm\infty$

(iii) $\|f(z)\|_+ \to 0$ as $\operatorname{Im} z \to \pm\infty$ in the strip, uniformly in $\operatorname{Re} z$.

Prove that $\mathscr{F}_\infty/(\mathscr{F}_\infty \cap K_t) = \mathscr{F}(X)/K_t$.

(d) Suppose that $h \in \mathscr{F}(X)$ and $h(z) = h(z + ia)$ for all $z \in S$. Define

$$y_n(t) = a^{-1} \int_0^a e^{-2\pi(t+is)n/a} h(t + is)\, ds$$

Show that $y_n(t) = y_n$ is independent of t, $y_n \in X_0 \cap X_1$, and

$$\frac{1}{N} \sum_{m=1}^{N} \sum_{n=-m}^{m} y_n e^{2\pi i n z/a} \xrightarrow{\|\|\cdot\|\|} h(z)$$

where the convergence is uniform with respect to y in $\|\cdot\|^{(1)}$ for $z = 1 + iy$ and in $\|\cdot\|^{(0)}$ for $z = iy$.

(e) Show that the set of functions in $\mathscr{F}_\infty$ of the form $e^{\beta z^2}(\sum_{n=1}^{N} x_n e^{\alpha_n t})$ where $x_n \in X_0 \cap X_1$, with $\beta > 0$, α_n, and N arbitrary, is dense in $\mathscr{F}_\infty$. (*Hint*: Since $e^{2\beta z^2} f \xrightarrow{\beta \to 0} f$ we need only look at functions of the form $g = e^{2\beta z^2} f$. Let $h = e^{\beta z^2} f$ and show that

$$h_n(z) = \sum_{m=-\infty}^{\infty} h(t + inm)$$

is a well-defined periodic element of $\mathscr{F}(X)$. Then, use (d) and the statement $\lim_{n\to\infty} e^{\beta z^2} h_n = g$.)

(f) Conclude that $X_t = \tilde{X}_t$.

38. (a) Let $\{\varphi_n\}$ be an orthonormal set (not necessarily complete) in a Hilbert space $\mathscr{H}$. Show that if C is a compact operator on $\mathscr{H}$, then $\|C\varphi_n\| \to 0$.

(b) Let $F \in L^1(\mathbb{R}^n, dx)$ and define

$$(A\varphi)(x) = \int_{\mathbb{R}^n} F(x - y)\varphi(y)\, dy$$

Prove that A is not compact unless F is the zero function.

39. (a) Let $f \in L^p_w$; $g \in L^{p'}_w$ where $p^{-1} + (p')^{-1} = 1$. Suppose that q satisfies $q^{-1} + p^{-1} < 1$. Then for all $h \in L^q$, prove that

$$\|f(g * h)\|_q \leq C_{p,q} \|f\|_{p,w} \|g\|_{p',w} \|h\|_q$$

(b) Let $0 < s < n/q$. Let $|p|$ be the operator $\sqrt{-\Delta}$ on $L^q(\mathbb{R}^n)$. Show that $|x|^{-s}|p|^{-s}$ defines a bounded map of $L^q(\mathbb{R}^n)$ into itself.

40. Let $N(h, f)$ be the operator $g \to h(f * g)$ on $L^2(\mathbb{R}^n)$.
(a) Prove that $N(h, f) \in \mathscr{I}_2$ if $h, f \in L^2$, and $\|N(h, f)\|_{\mathscr{I}_2} \leq \|h\|_2 \|f\|_2$.
(b) Prove that $\|N(h, f)\|_{\text{op}} \leq \|h\|_p \|f\|_q$ if $p^{-1} + q^{-1} = 1$ and $p \geq 2$.
(c) Prove that $N(h, f)$ is compact if $h \in L^p$, $g \in L^q$, $2 \leq p < \infty$.
(d) If $f \in L^1 \cap L^2$, prove that $N(f, h) \in \mathscr{I}_p$ if $h \in L^p$, $2 \leq p < \infty$. (*Hint*: Use interpolation.)

†41. This problem outlines the complex variables argument in the Malgrange–Ehrenpreis theorem.
(a) Let $f(z)$ be an analytic function of one complex variable on the disk $|z| \leq 1$ and let $p(z) = a_m z^m + a_{m-1} z^{m-1} + \cdots + a_0$. Prove that

$$|a_0 f(0)| \leq (2\pi)^{-1} \int_0^{2\pi} |f(e^{i\theta}) p(e^{i\theta})| \, d\theta$$

(*Hint*: Let $q(z) = (\prod_j (\bar{z}_j z - 1)/(z - z_j)) p(z)$ where the z_j are the zeros of f inside the unit circle. Notice that q is analytic on the disk and $|q(z)| = |p(z)|$ for $|z| = 1$.)
(b) Let f and p be as in part (a) and prove that

$$|a_k f(0)| \leq \frac{m!}{k!\,(m-k)!} (2\pi)^{-1} \int_0^{2\pi} |f(e^{i\theta}) p(e^{i\theta})| \, d\theta$$

(c) Let $F(\zeta)$ be an entire function of n complex variables and let $p(\zeta)$ be a polynomial of degree n. Suppose that $g(\zeta)$ is a nonnegative integrable function with compact support depending only on the absolute values $|\zeta_i|$, $i = 1, \ldots, n$. Prove that

$$|F(0) D^\alpha p(0)| \int_{\mathbb{C}^n} |\zeta|^\alpha g(\zeta) \, d\zeta \leq C_0 \int_{\mathbb{C}^n} |F(\zeta) p(\zeta)| g(\zeta) \, d\zeta$$

($d\zeta$ denotes Lebesgue measure on $\mathbb{C}^n$ and C_0 is a constant depending on α and m.)
(d) Use part (c) to prove the statement

$$|\tilde{q}(x) \hat{\varphi}(x)| \leq C_1 \int_{|\zeta| \leq \varepsilon} |\hat{\varphi}(x + \zeta) q(x + \zeta)| \, d\zeta$$

in the proof of the Malgrange–Ehrenpreis theorem.
Reference: K. Yosida, *Functional Analysis*, Springer, Berlin, 1965, pp. 185–186.

42. Find explicitly a fundamental solution for the ordinary differential equation $u'' = f$.

43. What do the regularity theorems of Section 6 say about the regularity of eigenfunctions of atomic Hamiltonians?
References: T. Kato, *Comm. Pure Appl. Math.* **10** (1957), 151–171; Section XIII.10 in Volume III of this series.

44. (a) Define the operation $\bar{\partial}$ on the C^∞ functions from $\mathbb{C}$ to $\mathbb{C}$ by $\bar{\partial} f = \partial f/\partial x + i \, \partial f/\partial y$ where $z \in \mathbb{C}$ is written $z = x + iy$. Prove that $\bar{\partial} f = 0$ is a restatement of the Cauchy–Riemann equations.
(b) Let $T \in \mathscr{D}'_{\mathbb{R}^2}$ where $\mathbb{C}$ is thought of as $\mathbb{R}^2$ and let $\bar{\partial} = \partial/\partial x + i \, \partial/\partial y$. Prove that if $\bar{\partial} T = 0$, then T is actually an analytic function. (*Hint*: Prove that $\Delta T = 0$ and apply the elliptic regularity theorem.)
(c) Let $T \in \mathscr{D}_{\mathbb{R}^{2n}}$ and suppose $\bar{\partial}_j T = 0$ for all $j = 1, 2, \ldots, n$. Prove that T is analytic.

45. (a) Prove that if Ω is a bounded open set and $V \in C^m(\Omega)$, $u \in W_k(\Omega)$ with $k \leq m$, then $Vu \in W_k(\Omega)$.
(b) Prove that if u is a weak solution of $-\Delta u + Vu = Eu$ and $V \in C^m(\Omega)$, then $u \in C^\ell(\Omega)$ for $\ell < m - \frac{1}{2}n + 2$.

*46. Using Sobolev's inequality (IX.19), prove the L^p Sobolev imbedding theorem; i.e. if $q^{-1} = p^{-1} - n\alpha^{-1}$ ($\alpha > 0$, $1 < p, q < \infty$) and if $f \in L^p$, then $g = \widehat{(1 + k^2)^{-\alpha} \hat{f}} \in L^q$.

47. Suppose that $f \in L^2(\mathbb{R}^3)$ and $\partial f/\partial x_i \in L^2(\mathbb{R}^3)$ for $i = 1, 2, 3$. Prove that $f \in L^p(\mathbb{R}^3)$ for all $p < 6$. (*Hint*: Use the Plancherel theorem, the function $(1 + |k|^2)^d$, and the Hausdorff–Young theorem.)

48. Let $\{f_\alpha\}_{|\alpha| \le m}$ be a family of $C^{|\alpha|}$ functions on $\mathbb{R}^n$. Let T and S be the differential operators

$$T\varphi = \sum_{|\alpha| \le m} \bar{f}_\alpha D^\alpha \varphi, \qquad S\varphi = \sum_{|\alpha| \le m} (-1)^{|\alpha|} D^\alpha (f_\alpha \varphi)$$

Let $T_{\min}$ denote the operator T defined on $C_0^\infty(\mathbb{R}^n)$ and let $T_{\max}$ be T defined on $\{\varphi \mid \varphi \in L^2(\mathbb{R}^n),\ T\varphi \in L^2(\mathbb{R}^n)\}$. Similarly, define $S_{\min}$ and $S_{\max}$.

(a) Prove that $S_{\min}^* = T_{\max}$, $T_{\min}^* = S_{\max}$.

(b) Prove that $T_{\min}$ is essentially self-adjoint if and only if both $T_{\min} = S_{\min}$ and $T_{\max}$ is self-adjoint.

Remark: When $T_{\min} = S_{\min}$, one says that T is *formally self-adjoint*. It may happen that $T_{\min}$ is formally self-adjoint but not even essentially self-adjoint, e.g. $-\Delta - x^4$ on $\mathbb{R}^n$. This is further discussed in the Appendix to Section X.1 and in Section X.5.

49. Let $H_n(x; \kappa) = \mathscr{F}^{-1}((\lambda^2 + \kappa^2)^{-1})$. Thus $G_0(x, y) = H_n(x - y; \kappa)$ is the free Green's function on $\mathbb{R}^n$. Suppose that $\kappa > 0$.

(a) Prove that $H_n(x; \kappa) = \kappa^{n-2} H_n(x\kappa; 1)$.

(b) Prove that

$$H_n(x; 1) = (4\pi)^{-n/2} \int_0^\infty e^{-\delta} e^{-|x|^2/4\delta} \frac{d\delta}{\delta^{n/2}} \tag{IX.68}$$

Hint: Use the form of the free propagator and the relation

$$(H_0 + 1)^{-1} = \int_0^\infty e^{-t} e^{-tH_0}\, dt$$

(c) Prove that $H(x; 1)$ is monotone decreasing in x and positive and that for $n \ge 3$,

$$H_n(x; 1) \le |x|^{2-n}$$

(d) If $n \ge 3$, prove that

$$\lim_{|x| \to 0} |x|^{n-2} H_n(x; 1) = (4\pi)^{-n/2} \int_0^\infty e^{-1/4y} \frac{dy}{y^{n/2}}$$

(*Hint for* (c) *and* (d): Let $y = \delta/|x|^2$.)

(e) Prove that $\lim_{|x| \to \infty} e^{|x|} |x|^{n/2 - 1/2} H_n(x; 1)$ exists and is nonzero. (*Hint*: Let $y = 2\delta/|x|$.)

50. (a) Let $T_\alpha = |x|^{-\alpha} \in \mathscr{S}'(\mathbb{R}^n)$ with $0 < \alpha < n$. Prove that $\hat{T}_\alpha$ is a C^∞ function on $\mathbb{R}^n \backslash \{0\}$ with $\hat{T} \circ R = \hat{T}$ for any rotation and $\hat{T} \circ D_\lambda = \lambda^{-n+\alpha} \hat{T}$ where D_λ is given in Problem 3. Conclude that

$$\widehat{|x|^{-\alpha}}(k) = C_{\alpha, n} |k|^{-n+\alpha}$$

(b) Let $T_{\alpha,\lambda} = (|k|^2 + \lambda^2)^{-\alpha/2}$, $0 < \alpha < n$, on $\mathbb{R}^n$. Prove that $\hat{T}_{\alpha,\lambda} \to \hat{T}_{\alpha,0}$ as $\lambda \to 0$ uniformly on compact subsets of $\mathbb{R}^n \backslash \{0\}$. Prove that $\hat{T}_{\alpha,\lambda} = \lambda^{-n+\alpha} \hat{T}_{\alpha,1} \circ D_{\lambda^{-1}}$ and conclude that $|k|^{n-\alpha} \hat{T}_{\alpha,1}(k)$ is bounded on the unit ball.

(c) Prove that $\hat{T}_{\alpha,1}(k)$ falls off exponentially and conclude that $\hat{T}_{\alpha,1}(k) \in L^{n/n-\alpha}_w$.

51. Let $\varphi \in \mathscr{S}(\mathbb{R}^n)$ and let $\alpha > 0$. Prove that there is a constant $C_{\alpha,\varphi}$, so that

$$\sup_{|x|\leq 1} \left| \left(\frac{x}{t}\right)^{\alpha} (e^{-iH_0 t}\varphi)(x) \right| \leq C_{\alpha,\varphi}\, t^{-n/2} \qquad \text{for} \quad t > 1$$

Reference: J. Kupsch and W. Sandas: "Møller Operators for Scattering on Singular Potentials," *Comm. Math. Phys.* **2** (1966), 147–154.

52. Let $H_0 = -\Delta$ on $\mathbb{R}^n$.
(a) Prove that $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n\backslash 0)$ if $n \geq 4$.
(b) Suppose that $n \leq 3$ and $A = -\Delta \restriction C_0^\infty(\mathbb{R}^n\backslash 0)$. Let $\varphi = \widehat{(\lambda^2 - i)^{-1}}$. Prove that $\varphi \in D(A^*)$ and that $A^*\varphi = i\varphi$. Conclude that $-\Delta$ is not essentially self-adjoint on $C_0^\infty(\mathbb{R}^n\backslash 0)$ if $n \leq 3$.

53. Use the Källen–Lehmann representation to prove that a quantum field $\varphi(x)$ cannot be a well-defined operator-valued *function* on $\mathbb{R}^4$. (*Hint*: Prove that $(\psi_0, \varphi(x)\varphi(y)\psi_0)$ is a bounded function, so that $\varphi(f)\psi_0 = 0$ for all $f \in \mathscr{S}(\mathbb{R}^4)$, thus violating the cyclicity of ψ_0.)

54. Let $f_n \to f$ in $\mathscr{S}(\mathbb{R}^4)$. Let $\psi \in D$. Prove that properties 3 and 4 of Section IX.8 imply that $\langle f, g\rangle \mapsto \langle \psi, \varphi(f)\varphi(g)\psi\rangle$ is jointly continuous. Conclude from this that $\varphi(f_n)\psi \to \varphi(f)\psi$.

55. (a) Let $g \in C_0^\infty(\mathbb{R}^n)$, with $\int_{-\infty}^{\infty} g(x_1, x_2, \ldots, x_n)\, dx_1 = 0$ for each fixed $\langle x_2, \ldots, x_n\rangle \in \mathbb{R}^{n-1}$. Prove that $g = \partial h/\partial x_1$ for some $h \in C_0^\infty(\mathbb{R}^n)$.
(b) Let $T \in \mathscr{D}'(\mathbb{R}^n)$ with $T(x_1 + a, x_2, \ldots, x_n) = T(x_1, x_2, \ldots, x_n)$ for all a in the sense that $T(U_a f) = T(f)$ for all $f \in \mathscr{D}(\mathbb{R}^n)$ where $(U_a f)(x_1, \ldots, x_n) = f(x_1 - a, \ldots, x_n)$. Prove there exists $S \in \mathscr{D}'(\mathbb{R}^{n-1})$ with

$$T(x_1, x_2, \ldots, x_n) = S(x_2, \ldots, x_n)$$

in the sense that $T(f) = S(I_1(f))$ for all $f \in \mathscr{D}(\mathbb{R}^n)$ where $(I_1(f))(x_2, \ldots, x_n) = \int f(x_1, \ldots, x_n)\, dx_1$. (*Hint*: Choose $F \in \mathscr{D}(R)$ with $\int F(t)\, dt = 1$. Recall from Problem 47 of Chapter V that $\partial T/\partial x_1 = 0$. Finally use (a) to prove that

$$g = f - F(x_1)I_1(f) = \partial h/\partial x_1)$$

(c) Let T and S be as in (b). Prove that if T is tempered, then S is tempered.

56. The goal of this problem is to prove that any tempered distribution T with support in $\overline{V}_+ \cup (-\overline{V}_+)$ can be written $T = R + A$ where supp $R \subset \overline{V}_+$ and supp $A \subset -\overline{V}_+$.
(a) Let f be a C^∞ function on the unit sphere S in $\mathbb{R}^4$ with $f = 1$ on $\overline{V}_+ \cap S$ and $f = 0$ on $-\overline{V}_+ \cap S$. Let $\chi(\mathbf{x}) = f(\mathbf{x}/|\mathbf{x}|)$. Show that $(x^2)^n\chi(\mathbf{x})$ is a C^{2n-1} function.
(b) Suppose that $|T(g)| \leq \sum_{|\alpha|\leq N,\, |\beta|\leq M} \|x^\alpha D^\beta g\|_\infty$. Prove that $(x^2)^{M+1}T$ can be written as $S_+ + S_-$ where supp $S_+ \subset \overline{V}_+$ and supp $S_- \subset -\overline{V}_+$. (*Hint*: Let $S_+(f) = T[(x^2)^{M+1}\chi f]$.)
(c) Pick a fixed h in $C_0^\infty(\mathbb{R}^4)$, with $h \equiv 1$ near $x = 0$. Let

$$Hf = (x^2)^{-M-1}\left[f - \sum_{|\beta|\leq 2M+1} \frac{(D^\beta f)(0)}{\beta!}\, x^\beta h\right]$$

Prove that $T(f) = (x^2)^{M+1}T(Hf) + T_0$ where T_0 has support at the origin.

†57. Prove Theorem IX.38 for the case of codimension greater than one.

†58. Fill in the details of the proof of Theorem IX.40.

59. Give an example of a tempered distribution T given by a polynomially bounded C^∞ function F so that the family of translates $\{T_x\}$ is bounded as a family of distributions but such that F is *not* a bounded function. (*Hint*: Modify Example 1 of Section IX.10).

†60. Complete the proof of Theorem IX.43.

61. Let $T, S \in \mathscr{D}'(\mathbb{R})$ so that the products TS, $T'S$, and TS' all exist. Prove that $(TS)' = T'S + TS'$.

62. Let C be a convex cone in $\mathbb{R}^n$ with nonempty interior. Let $\mathscr{A}$ be the family of functions analytic in $\mathbb{R}^n + iC$, polynomially bounded at infinity and as $\operatorname{Im} z \downarrow 0$. For $F \in \mathscr{A}$, let $BV(F)$ denote the distributional boundary value of F. If $F, G \in \mathscr{A}$, prove that the product $BV(F)BV(G)$ exists and that

$$BV(F)BV(G) = BV(FG)$$

63. For any $T \in \mathscr{D}'(\mathbb{R}^n)$ and any $\alpha \in I_+^n$ prove that $WF(D^\alpha T) = WF(T)$.

64. (a) For any $T \in \mathscr{D}'(\mathbb{R}^n)$ and $f \in \mathscr{D}(\mathbb{R}^n)$, prove that

$$WF(fT) \subset \{\langle x, k\rangle \mid x \in \operatorname{supp} f; \langle x, k\rangle \in WF(T)\}$$

and that

$$WF(fT) \supset \{\langle x, k\rangle \mid f(x) \neq 0; \langle x, k\rangle \in WF(T)\}$$

(b) Give an example of f, T as in part (a) for which

$$WF(fT) \neq \{\langle x, k\rangle \mid x \in \operatorname{supp} f; \langle x, k\rangle \in WF(T)\}$$

*65. (a) Define the asymptotic conical support $ACS(T)$ of a distribution T as the complement of those $k \neq 0$ for which there exists a neighborhood N and a Λ_0 so that $\operatorname{supp} T \cap \lambda N = \varnothing$ if $\lambda > \Lambda_0$. Prove that $ACS(T)$ is a closed cone.

(b) Prove that for $T \in \mathscr{S}'(\mathbb{R}^n)$, $WF_x(T) \subset ACS(\hat{T})$ for any $x \in \mathbb{R}^n$.

(c) Without using the machinery of oscillatory integrals, obtain enough information about $WF(\Delta_+)$ to prove that the product $\theta\Delta_+$ exists.

66. †(a) Prove Theorem IX.46.

(b) Refine Theorem IX.46 by finding necessary and sufficient conditions on F, an asymptotic symbol of order k, so that $\operatorname{sing\,supp}(\hat{F}) = \varnothing$.

67. Define $\operatorname{Sym}(\Omega, s, m, \rho, \delta)$ as $\operatorname{Sym}(\Omega, s, m)$ was defined but with (IX.63) replaced by

$$|(D_x^\alpha D_\theta^\beta a)(x, \theta)| \leq d(1 + |\theta|)^{m - \rho|\beta| + \delta|\alpha|}$$

Extend Theorem IX.49 to the case $\delta < 1$, $\rho > 0$.

†68. Prove that

$$a(x, \theta; m) = (m^2 + |\theta|^2)^{-1/2} \exp(-ix_0[(m^2 + |\theta|^2)^{1/2} - |\theta|])$$

is an asymptotic symbol of order -1.

†69. Prove Lemmas 1 and 2 in the proof of Theorem IX.47.

†70. Prove that the map V used in the proof of Theorem IX.47 maps $\mathrm{Sym}(\Omega, s, m)$ continuously to $\mathrm{Sym}(\Omega, s, m-1)$.

†71. Prove that $\langle a, f\rangle \to af$ is a continuous bilinear map of $\mathrm{Sym}(\Omega, s, m) \times C_0^\infty(\Omega)$ to $\mathrm{Sym}(\Omega, s, m)$.

†72. Complete the proof of (c) of Theorem IX.48. *Hint*: Show that

$$t^n \exp(i\omega(k)t) = \left[\frac{\omega(k)}{i|k|^2}(\mathbf{k}\cdot\nabla_k)\right]^n e^{i\omega(k,t)}$$

where $\omega(k) = \sqrt{m^2 + k^2}$.

†73. Under the situation described in the notes to Section IX.10, prove that $WF(f\delta_F) \subset N(F)$ and that $WF(\delta_F) = N(F)$.

†74. Find two distributions T, S of compact support so that TS exists but $\int \hat{T}(\ell)\hat{S}(k-\ell)\,d\ell$ diverges absolutely for all k.

†,*75. The purpose of this problem is to prove the change of variables formula in (f) of Theorem IX.44.

(a) Verify the formula when M is a linear transformation.

(b) Show that it is enough to prove that

$$WF_{x=0}(T \circ M) = WF_{x=0}(T)$$

whenever M is a diffeomorphism with $M(0) = 0$ and $dM_{x=0}$ = identity map and T is a distribution of compact support.

(c) Prove that if $g \in C_0^\infty(\mathbb{R}^n)$, then

$$\widehat{g(T\circ M)}(\ell) = (2\pi)^{-n}\iint g(x)\hat{T}(k)\exp[i(k\cdot M(x) - \ell\cdot x)]\,dx\,dk$$

in the sense that the integral formula is correct if $(1+k^2)^{n+1/2}\hat{T}(k)$ is bounded and for fixed ℓ, the map

$$T \mapsto \text{integral}$$

is continuous in the norm $\|T\|_m = \sup_k\|(1+k^2)^{-m}\hat{T}(k)\|$ for each $m > 0$. (*Hint*: Use the integration by parts machine based on $|(dM_x^*)^{-1}\,\mathrm{grad}_x(k\cdot M(x))| = |k|$.)

(d) Suppose k_0 is a unit vector with $k_0 \notin WF_{x=0}(T)$. Show that under the conditions in (b) one can pick open cones C_0 and C_1 about k_0 and a neighborhood N of $x = 0$ so that: (i) For every m,

$$\sup_{k\in C_1}(1+k^2)^m|\widehat{gT}(k)| < \infty$$

for any g with $\mathrm{supp}\, g \subset N$.

(ii) $\quad \sup\{\ell\cdot[dM_x^*(k)]\,|\,\ell\in C_0, k\notin C_1, x\in N; |\ell| = |k| = 1\} = \alpha < 1$

(e) Prove that for any m,

$$\sup_\ell\left|(1+\ell^2)^m\int_{k\in C_1} g(x)\hat{T}(k)\exp[i(k\cdot M(x) - \ell\cdot x)]\,dx\,dk\right|$$

is finite. (*Hint*: Use (i) of (d) and the integration by parts machine based on $\ell^2\exp(-i\ell\cdot x) = -\Delta_x[\exp(-i\ell\cdot x)]$.)

(f) Let

$$F(k, \ell) = \int g(x) \exp[i(k \cdot M(x) - \ell \cdot x)]\, dx$$

Prove that for any $m > 0$

$$\sup\{(1 + \lambda^2)^m F(\lambda k_0, \lambda \ell_0) \mid k_0 \notin C_1, \ell_0 \in C_0, |k_0 + \ell_0| = 1\} < \infty$$

Hint: Use (ii) of (d) and the integration by parts machine based on

$$|dM_x^*(k) - \ell|^{-2}\{(dM_x^*(k) - \ell) \cdot \operatorname{grad}_x[k \cdot M(x) - \ell \cdot x]\} = 1$$

(g) Prove that $\sup_{k \notin C_1, \ell \in C_0} (1 + |k| + |\ell|)^m F(k, \ell) < \infty$ for all m and conclude that $k \notin WF_{x=0}(T \circ M)$.

(h) Use symmetry and the result $WF_{x=0}(T \circ M) \subset WF_{x=0}(T)$ just proven to conclude the proof.

†76. The purpose of this problem is to outline the proofs of Theorems IX.13 and IX.14.

(a) Prove that $e^{b|x|} f \in L^2$ for all $b < a$ if and only if $e^{\eta \cdot x} f \in L^2$ for all $\eta \in \mathbb{R}^n$ with $|\eta| < a$.

(b) If $e^{b|x|} f \in L^2$ for all $b < a$, prove that $\hat{f}(\cdot)$ has an analytic continuation to $\{z \| \operatorname{Im} z| < a\}$ and that $\hat{f}(\cdot + i\eta) = \widehat{e^{\eta \cdot x} f}$. Conclude that the bound in Theorem IX.13 holds.

(c) Suppose that $\hat{f}$ has an analytic continuation to the tube $\{z \| \operatorname{Im} z| < a\}$ with the given bound. Use the Cauchy integral theorem to prove that for any $g \in C_0^\infty(\mathbb{R}^n)$ and $\eta \in \mathbb{R}^n$ with $|\eta| < a$,

$$\int \overline{g(x)} f(x)\, dx = \int \overline{\hat{g}(k - i\eta)} \hat{f}(k + i\eta)\, dk$$

(d) Prove that if f obeys the hypotheses of (c) and if $h_\eta = \hat{f}(\cdot + i\eta)$, then $\widetilde{h_\eta(x)} = e^{\eta \cdot x} f$ almost everywhere and so conclude the proof of Theorem IX.13.

(e) By mimicking the above, prove Theorem IX.14.

77. (a) Use Hunt's interpolation theorem to prove that if $p^{-1} + q^{-1} = r^{-1}$, p and q less than ∞, $r > 1$, and if $f \in L^p(\mathbb{R}^n)$, $g \in L^q_w(\mathbb{R}^n)$, then $fg \in L^r_w(\mathbb{R}^n)$.

(b) Show that *if* the Marcinkiewicz interpolation theorem held without the restriction $p_i \le q_i$, then it would follow that $f \in L^4(\mathbb{R}^n)$ and $g \in L^4_w(\mathbb{R}^n)$ implies that $fg \in L^2(\mathbb{R}^n)$.

(c) Find explicit functions $f \in L^4(\mathbb{R}^n)$ and $g \in L^4_w(\mathbb{R}^n)$ so that $fg \notin L^2(\mathbb{R}^n)$.

78. (the uncertainty principle) Let $P = -i\hbar(d/dx)$ and $Q = x$ be operators on $L^2(\mathbb{R})$. Let $\varphi \in \mathscr{S}(\mathbb{R})$ with $\|\varphi\| = 1$ and define:

$$m_p = (P\varphi, \varphi), \qquad m_q = (Q\varphi, \varphi)$$
$$\sigma_p^2 = \|(P - m_p)\varphi\|^2, \qquad \sigma_q^2 = \|(Q - m_q)\varphi\|^2$$

(a) Using the commutation relation $PQ - QP = -i\hbar$, prove that $\sigma_p \sigma_q \ge \hbar/2$.

(b) Restate the result of part (a) in terms of μ_q and μ_p, the spectral measures of φ for Q and for P, and explain what this means for measurements of position and momentum in quantum mechanics (see Section VIII.11).

(c) Reformulate the result of part (a) as a statement about the Fourier transform.

READER'S GUIDE

Chapter IX is essentially self-contained and the prerequisites for it are minimal. The reader should know the properties of the Lebesgue integral, the elementary notions of Hilbert and Banach spaces, and the definition and basic properties of the Schwartz space of rapidly decreasing functions and its dual, the tempered distributions. This material is covered in Chapters I–III and Sections V.1–V.3 of Volume I and in many other functional analysis texts. The occasional reference to theorems in Volume I is usually descriptive so that the reader familiar with another elementary text can understand the reference.

We give a section by section description below. Here is a summary: The most basic material in Chapter IX is in Sections 1, 2, and the first part of 3. The reader mainly interested in quantum mechanics should consult especially Sections 1, 2, the first part of 3, 4, 7, and have some acquaintance with Section 9 and the Appendix to Section 4. The reader interested in quantum field theory should consult Sections 1, 2, 3, and 8. For partial differential equations, he should consult Sections 1, 2, the first part of 3, 4, 5, 6, and 10.

The fundamental properties of the Fourier transform are presented in Sections 1, 2, 4, and the first part of 3. In Section 1, the Fourier transform is defined on $\mathscr{S}(\mathbb{R}^n)$ and extended to $\mathscr{S}'(\mathbb{R}^n)$ by the adjoint map. The Fourier inversion theorem is proven, and we define and investigate the properties of convolution. In Section 2 we study the range of the Fourier transform on the classical spaces, proving the Plancherel, Hausdorff–Young, and Bochner theorems. In the first part of Section 3 we prove the Paley–Wiener theorems characterizing the Fourier transforms of C^∞ functions and distributions with compact support. In the second part of Section 3 we prove a more difficult theorem characterizing the Fourier transforms of tempered distributions in $\mathbb{R}^4$ with supports in cones. The reader should skip this part on first reading unless he is interested in the Wightman axioms (Section 8). Finally, in Section 4 we present various L^p-estimates relating Fourier transforms and convolutions. The reader should know how to use the interpolation theorems given in the Appendix since they are the basic tool for proving the estimates. The idea of interpolation is beautiful, but the proofs of the interpolation theorems are involved, so the proofs in the Appendix should be skipped on first reading.

The remaining sections, 5–10, deal with more advanced material and applications. Sections 5 and 6 present applications of the Fourier transform to partial differential equations. In Section 5 we prove the existence of fundamental solutions for constant coefficient partial differential equations. In Section 6 we investigate the Sobolev spaces and prove that every weak solution of $\Delta u = f$ is in fact a strict solution (Weyl's lemma).

In Section 7, we use the Fourier transform to derive properties of the free quantum-mechanical Hamiltonian $H_0 = -\Delta$, its resolvent $(H_0 + \kappa^2)^{-1}$, and the group it generates e^{-iH_0t}.

In Section 8, we present and discuss the Gårding–Wightman axioms for a Hermitian scalar quantum field theory. No previous acquaintance with quantum field theory is necessary for reading this section. We show how the Fourier transform may be used to determine the analytic continuation properties of the Wightman function and to prove the PCT theorem. The technical appendix is devoted to proving a representation formula for polynomially bounded, Lorentz invariant measures with support in the closed forward light cone.

In Section 9, we consider the question of which L^2 functions on $\mathbb{R}^n$ have a natural restriction to a lower dimensional submanifold. This material will not be applied until we investigate the spectrum of quantum mechanical Hamiltonians in Chapter XIII. On first

reading, the statement of Theorem IX.41 and the general idea of its proof should be understood, but the gory details should be omitted.

Section 10 is intended as an introduction to wave front sets and oscillatory integrals, two important tools for the study of partial differential equations with nonconstant coefficients. This theory can be used to give conditions on two distributions so that their product is well defined. The material in Section 10 is not used again in Volumes II and III.

X: Self-Adjointness and the Existence of Dynamics

People used to think that when a thing changes, it must be in a state of change and that when a thing moves, it is in a state of motion. This is now known to be a mistake. *B. Russell*

X.1 Extensions of symmetric operators

We begin this chapter by studying symmetric operators and their extensions. Primarily, we wish to answer two questions: When do symmetric operators have self-adjoint extensions and, if they do, how can the extensions be characterized? These questions are answered by von Neumann's theory of deficiency indices which we will develop using many of the techniques we have already used in proving the basic criterion for self-adjointness (Theorem VIII.3) in Chapter VIII.

It is useful to begin by explaining why symmetric, non-self-adjoint operators are of interest in the first place. Typically, in quantum mechanics or quantum field theory, physical reasoning gives a formal expression for the Hamiltonian of the system; it is usually a partial differential operator on an appropriate L^2 space. We say "formal" when the domain of the Hamiltonian is not specified. It is usually easy to find a dense domain on which the formal Hamiltonian is a well-defined and symmetric operator H. The quantum dynamics should be given by a unitary group, and we know from Stone's theorem (Theorem VIII.8) that the infinitesimal generator of such a group must be self-adjoint. If $\overline{H}$, the closure of H, is self-adjoint,

then we can use H. But if H is not self-adjoint, then we must ask: Does H have self-adjoint extensions? And if it has several, which one shall we choose to generate the dynamics? In the case where there are several self-adjoint extensions, they are usually distinguished by the *physics* of the system being described. The problem of choosing the "right" self-adjoint extension is not just a mathematical "technicality" but is intimately related to the physics. For further discussion, see Examples 1 and 2 in this section.

We remark that throughout this section we discuss the extensions of *closed* symmetric operators. There is no loss of generality since every symmetric operator has a closure, and the operator and its closure have the same closed extensions.

Theorem X.1 Let A be a closed symmetric operator on a Hilbert space $\mathscr{H}$. Then

(1a) $\dim[\mathrm{Ker}(\lambda I - A^*)]$ is constant throughout the open upper half-plane.
(1b) $\dim[\mathrm{Ker}(\lambda I - A^*)]$ is constant throughout the open lower half-plane.

(2) The spectrum of A is *one* of the following:
  (a) The closed upper half-plane
  or (b) the closed lower half-plane
  or (c) the entire plane
  or (d) a subset of the real axis

(3) A is self-adjoint if and only if case (2d) holds.

(4) A is self-adjoint if and only if the dimensions in both (1a) *and* (1b) are zero.

Proof Let $\lambda = \nu + i\mu$, $\mu \neq 0$. Since A is symmetric,

$$\|(\lambda - A)\varphi\|^2 \geq \mu^2 \|\varphi\|^2 \tag{X.1}$$

for all $\varphi \in D(A)$. From this inequality and the fact that A is closed, it follows immediately that $\mathrm{Ran}(\lambda - A)$ is a closed subspace of $\mathscr{H}$. Furthermore,

$$\mathrm{Ker}(\lambda - A^*) = \mathrm{Ran}(\bar{\lambda} - A)^{\perp} \tag{X.2}$$

The proof of these statements are the same as the case $\lambda = i$ which is given in the proof of Theorem VIII.3.

We will show that if $\eta \in \mathbb{C}$ is small enough, $\mathrm{Ker}(\lambda - A^*)$ and $\mathrm{Ker}((\lambda + \eta) - A^*)$ have the same dimension. Let u in $D(A^*)$ lie in $\mathrm{Ker}((\lambda + \eta) - A^*)$ with $\|u\| = 1$. Suppose $(u, v) = 0$ for all $v \in \mathrm{Ker}(\lambda - A^*)$.

Then by (X.2) $u \in \text{Ran}(\bar{\lambda} - A)$, so there is a $\varphi \in D(A)$ with $(\bar{\lambda} - A)\varphi = u$. Thus,

$$0 = (((\lambda + \eta) - A^*)u, \varphi) = (u, (\bar{\lambda} - A)\varphi) + \bar{\eta}(u, \varphi)$$
$$= \|u\|^2 + \bar{\eta}(u, \varphi)$$

This is a contradiction if $|\eta| < |\mu|$ since by (X.1) $\|\varphi\| \leq \|u\|/|\mu|$. Thus for $|\eta| < |\mu|$, there is no $u \in \text{Ker}((\lambda + \eta) - A^*)$ which is in $\text{Ker}(\lambda - A^*)^\perp$. A short argument with projections (Problem 4) now shows that

$$\dim[\text{Ker}((\lambda + \eta) - A^*)] \leq \dim[\text{Ker}(\lambda - A^*)]$$

The same argument shows that if $|\eta| < |\mu|/2$, then $\dim[\text{Ker}(\lambda - A^*)] \leq \dim[\text{Ker}((\lambda + \eta) - A^*)]$, so we conclude that

$$\dim[\text{Ker}(\lambda - A^*)] = \dim[\text{Ker}((\lambda + \eta) - A^*)] \quad \text{if} \quad |\eta| < |\mu|/2$$

Since $\dim[\text{Ker}(\lambda - A^*)]$ is locally constant, it equals a constant in the upper half-plane and equals a (possibly different) constant in the lower half-plane. This proves (1).

It follows from (X.1) that if $\text{Im } \lambda \neq 0$, $\lambda - A$ always has a bounded left inverse and from (X.2) that the inverse is everywhere defined if and only if $\dim[\text{Ker}(\bar{\lambda} - A^*)] = 0$. Thus it follows from part (1) that each of the open upper and lower half-planes is either entirely in the spectrum of A or entirely in the resolvent set. This, plus the fact that $\sigma(A)$ is closed proves (2). (3) and (4) are restatements of Theorem VIII.3. ∎

Corollary If A is a closed symmetric operator that is semibounded, i.e. $(A\varphi, \varphi) \geq -M\|\varphi\|^2$, then $\dim[\text{Ker}(\lambda - A^*)]$ is constant for

$$\lambda \in \mathbb{C} \backslash [-M, \infty)$$

Proof This corollary follows from the proof of Theorem X.1. The same argument about the invariance of dimension can be carried out for real λ in $(-\infty, -M)$, thus connecting the upper and lower half-planes.

Corollary If a closed symmetric operator has at least one real number in its resolvent set, then it is self-adjoint.

Proof Since the resolvent set is open and contains a point on the real axis, it must contain points in both the upper and lower half-planes. The corollary now follows from part (3) of Theorem X.1.

Since the dimensions of the kernels of $i - A^*$ and $i + A^*$ play an important role, it is convenient to give them names.

Definition Suppose that A is a symmetric operator. Let

$$\mathscr{K}_+ = \mathrm{Ker}(i - A^*) = \mathrm{Ran}(i + A)^\perp$$
$$\mathscr{K}_- = \mathrm{Ker}(i + A^*) = \mathrm{Ran}(-i + A)^\perp$$

$\mathscr{K}_+$ and $\mathscr{K}_-$ are called the **deficiency subspaces** of A. The pair of numbers n_+, n_-, given by $n_+(A) = \dim[\mathscr{K}_+]$, $n_-(A) = \dim[\mathscr{K}_-]$ are called the **deficiency indices** of A.

We remark that it is possible for the deficiency indices to be any pair of nonnegative integers; and further it is possible for n_+ or n_- (or both) to equal infinity. The reader is asked to construct examples in Problem 1.

We now set about the task of constructing the closed symmetric extensions of A. Let B be such an extension. Then for $\varphi \in D(B^*)$, we have $(\psi, B^*\varphi) = (B\psi, \varphi) = (A\psi, \varphi)$ for all $\psi \in D(A)$. Thus $\varphi \in D(A^*)$ and $B^*\varphi = A^*\varphi$ so

$$A \subseteq B \subseteq B^* \subseteq A^* \tag{X.3}$$

We introduce two new sesquilinear forms on $D(A^*)$:

$$(\varphi, \psi)_A = (\varphi, \psi) + (A^*\varphi, A^*\psi)$$
$$[\varphi, \psi]_A = (A^*\varphi, \psi) - (\varphi, A^*\psi)$$

A subspace of $D(A^*)$ such that $[\varphi, \psi]_A = 0$ for all φ and ψ in the subspace will be called **A-symmetric**. When we refer to subspaces of $D(A^*)$ as **A-closed** or **A-orthogonal** we mean in the inner product given by the graph inner product $(\cdot, \cdot)_A$.

Lemma Let A be a closed symmetric operator. Then

(a) The closed symmetric extensions of A are the restrictions of A^* to A-closed, A-symmetric subspaces of $D(A^*)$.

(b) $D(A)$, $\mathscr{K}_+$, and $\mathscr{K}_-$ are A-closed, mutually A-orthogonal subspaces of $D(A^*)$ and

$$D(A^*) = D(A) \oplus_A \mathscr{K}_+ \oplus_A \mathscr{K}_-$$

(c) There is a one-to-one correspondence between A-closed, A-symmetric subspaces S of $D(A^*)$ which contain $D(A)$ and the A-closed, A-symmetric subspaces S_1 of $\mathscr{K}_+ \oplus_A \mathscr{K}_-$ given by $S = D(A) \oplus_A S_1$.

Proof To prove (a), notice that (X.3) implies that every symmetric extension of A is contained in A^*. Further, the extension is closed if and only if its domain is A-closed and the extension is symmetric if and only if its domain is A-symmetric.

To prove (b), notice that $D(A)$ is A-closed since A is closed, and $\mathscr{K}_+$ and $\mathscr{K}_-$ are A-closed since they are already closed in the weaker topology given by the usual inner product. The fact that the three subspaces are orthogonal is a straightforward calculation which we omit. Suppose $\psi \in D(A^*)$ and $\psi \perp_A D(A) \oplus_A \mathscr{K}_+ \oplus_A \mathscr{K}_-$. For $\varphi \in D(A)$, we have $(\varphi, \psi) + (A^*\varphi, A^*\psi) = (\varphi, \psi)_A = 0$, so

$$(\varphi, \psi) = -(A\varphi, A^*\psi)$$

Thus, $A^*\psi \in D(A^*)$ and $A^*A^*\psi = -\psi$. Since

$$(A^* + i)(A^* - i)\psi = (A^*A^* + I)\psi = 0,$$

we conclude that $(A^* - i)\psi \in \mathscr{K}_-$. But if $\varphi \in \mathscr{K}_-$, then

$$\begin{aligned} i(\varphi, (A^* - i)\psi) &= (\varphi, \psi) + (A^*\varphi, A^*\psi) \\ &= (\varphi, \psi)_A = 0 \end{aligned}$$

since $\psi \perp_A \mathscr{K}_-$. Thus, we must have $(A^* - i)\psi = 0$, which implies that $\psi \in \mathscr{K}_+$. Since $\psi \perp_A \mathscr{K}_+$, we conclude that $\psi = 0$ which completes the proof of (b).

Let S_1 be an A-closed, A-symmetric subspace of $\mathscr{K}_- \oplus_A \mathscr{K}_-$. Suppose that $\varphi = \varphi_0 + \varphi_1$, $\psi = \psi_0 + \psi_1$ with φ_0, $\psi_0 \in D(A)$; φ_1, $\psi_1 \in S_1$. Then $[\varphi_0, \psi_0]_A = 0$ since A is symmetric and $[\varphi_1, \psi_1]_A = 0$ since S_1 is A-symmetric. Further,

$$\begin{aligned} [\varphi_0, \psi_1]_A &= (A^*\varphi_0, \psi_1) - (\varphi_0, A^*\psi_1) \\ &= (A\varphi_0, \psi_1) - (\varphi_0, A^*\psi_1) \\ &= 0 \end{aligned}$$

since $\varphi_0 \in D(A)$ and $\psi_1 \in D(A^*)$. A similar proof shows that $[\varphi_1, \psi_0]_A = 0$. Thus,

$$[\varphi, \psi]_A = [\varphi_0, \psi_0]_A + [\varphi_1, \psi_0]_A + [\varphi_0, \psi_1]_A + [\varphi_1, \psi_1]_A = 0$$

so $S = D(A) \oplus_A S_1$ is an A-symmetric subspace. S is A-closed since $D(A)$ and S_1 are A-closed and A-orthogonal.

Conversely, let S be an A-closed, A-symmetric subspace of $D(A^*)$ containing $D(A)$. Let $S_1 = S \cap (\mathscr{K}_+ \oplus_A \mathscr{K}_-)$. Then S_1 is clearly A-closed and A-symmetric. Now suppose that $\varphi \in S$. Then φ can be uniquely expressed $\varphi = \varphi_0 + \varphi_1$ where $\varphi_0 \in D(A)$ and $\varphi_1 \in \mathscr{K}_+ \oplus_A \mathscr{K}_-$. Since $D(A) \subset S$, we have $\varphi_0 \in S$ which implies $\varphi_1 \in S$ also. Thus $\varphi_1 \in S_1$ so $S = D(A) \oplus_A S_1$. This proves (c). ∎

We are now ready to prove the main theorem of this section.

Theorem X.2 Let A be a closed symmetric operator. The closed symmetric extensions of A are in one-to-one correspondence with the set of partial isometries (in the usual inner product) of $\mathscr{K}_+$ into $\mathscr{K}_-$. If U is such an isometry with initial space $I(U) \subseteq \mathscr{K}_+$, then the corresponding closed symmetric extension A_U has domain

$$D(A_U) = \{\varphi + \varphi_+ + U\varphi_+ \,|\, \varphi \in D(A), \varphi_+ \in I(U)\}$$

and

$$A_U(\varphi + \varphi_+ + U\varphi_+) = A\varphi + i\varphi_+ - iU\varphi_+$$

If $\dim I(U) < \infty$, the deficiency indices of A_U are

$$n_\pm(A_U) = n_\pm(A) - \dim[I(U)]$$

Proof Let A_1 be a closed symmetric extension of A. From the lemma we know that $D(A_1) = D(A) \oplus_A S_1$ where S_1 is an A-closed A-symmetric subspace of $\mathscr{K}_+ \oplus \mathscr{K}_-$. If $\varphi \in S_1$, it can be written uniquely as $\varphi = \varphi_+ + \varphi_-$. Since S_1 is A-symmetric

$$\begin{aligned} 0 &= (A^*\varphi, \varphi) - (\varphi, A^*\varphi) \\ &= 2i(\varphi_-, \varphi_-) - 2i(\varphi_+, \varphi_+) \end{aligned}$$

which implies that

$$\|\varphi_+\|^2 = \|\varphi_-\|^2 \tag{X.4}$$

Since S_1 is a subspace of $\mathscr{K}_+ \oplus_A \mathscr{K}_-$, (X.4) shows that $\varphi_+ \mapsto \varphi_-$ is a well-defined isometry from a subspace of $\mathscr{K}_+$ into $\mathscr{K}_-$. Call the corresponding partial isometry U. Then

$$D(A_1) = \{\varphi + \varphi_+ + U\varphi_+ \,|\, \varphi \in D(A), \varphi_+ \in I(U)\} \tag{X.5}$$

and

$$A_1(\varphi + \varphi_+ + U\varphi_+) = A^*(\varphi + \varphi_+ + U\varphi_+) = A\varphi + i\varphi_+ - iU\varphi_+ \tag{X.6}$$

Conversely, let U be an isometry from a subspace of $\mathscr{K}_+$ into $\mathscr{K}_-$ and define $D(A_1)$ and A_1 by (X.5) and (X.6). Then $D(A_1)$ is an A-closed, A-symmetric subspace of $D(A^*)$, so by the lemma, A_1 is a closed symmetric extension of A.

The statement about deficiency indices follows by looking at the ranges of $i + A_1$ and $i - A_1$ on $D(A_1)$. ∎

Corollary Let A be a closed symmetric operator with deficiency indices n_+ and n_-. Then,

(a) A is self-adjoint if and only if $n_+ = 0 = n_-$.
(b) A has self-adjoint extensions if and only if $n_+ = n_-$. There is a one–one correspondence between self-adjoint extension of A and unitary maps from $\mathscr{K}_+$ onto $\mathscr{K}_-$.
(c) If either $n_+ = 0 \neq n_-$ or $n_- = 0 \neq n_+$, then A has no nontrivial symmetric extensions (such operators are called **maximal symmetric**).

Example 1 We will consider the example introduced in Section VIII.2 from several points of view. Let T be the operator $i\,d/dx$ on $L^2(0, 1)$ with the domain $D(T) = \{\varphi \mid \varphi \in AC[0, 1], \varphi(0) = 0 = \varphi(1)\}$. We showed in Section VIII.2 that T^* is the operator $i\,d/dx$ with domain $D(T^*) = AC[0, 1]$.

Since the operator T is so simple and since we know the domain of its adjoint explicitly, we can determine the self-adjoint extensions of T without using the machinery developed in this section. It is instructive to do that first. Suppose S is a symmetric extension of T. Since $D(S^*) \subset D(T^*)$, we know that the functions in $D(S^*)$ are absolutely continuous and $S^*\varphi = i\,d\varphi/dx$. Thus for $\varphi \in D(S)$ and $\psi \in D(S^*)$, integration by parts shows that

$$(S\varphi, \psi) - (\varphi, S^*\psi) = \overline{\varphi(1)}\psi(1) - \overline{\varphi(0)}\psi(0) = 0 \tag{X.7}$$

In the case $S = T$ we can see why T is not self-adjoint. The boundary conditions on the functions in $D(T)$ are so strong that no boundary conditions on the functions in $D(T^*)$ are necessary in order to ensure that the right-hand side of (X.7) equals zero. What is necessary is to extend the set of functions in $D(S)$ by allowing more general boundary conditions so that the equality (X.7) requires the *same* boundary conditions on the functions in $D(S^*)$. We now do this. Let S be a self-adjoint extension of T and suppose that $\varphi \in D(S)\backslash D(T)$. Then (X.7) requires that $|\varphi(1)|^2 = |\varphi(0)|^2$ and since $\varphi \notin D(T)$, $\varphi(0) \neq 0$, so there is an α with $|\alpha| = 1$ so that $\varphi(1) - \alpha\varphi(0) = 0$. If ψ is any other function in $D(S)$, then (X.7) requires that $\psi(1) = \alpha\psi(0)$ with the *same* α. Thus, $S \subset T_\alpha$ where $T_\alpha = i\,d/dx$ on

$$D(T_\alpha) = \{\varphi \mid \varphi \in AC[0, 1], \varphi(1) = \alpha\varphi(0)\}$$

Since T_α is symmetric and S is self-adjoint, $S = T_\alpha$ for some α.

Next, we determine which T_α are self-adjoint. Choose $\varphi \in D(T_\alpha)$ and $\psi \in D(T_\alpha^*)$. Then (X.7) requires that

$$\bar{\alpha}\,\overline{\varphi(0)}\psi(1) - \overline{\varphi(0)}\psi(0) = 0$$

so that $\psi(1) = \alpha\psi(0)$. Thus $\psi \in D(T_\alpha)$, so $D(T_\alpha^*) = D(T_\alpha)$, i.e. T_α is self-adjoint for each α. Thus, the set of self-adjoint extensions of T consists of the collection of operators $\{T_\alpha | \alpha \in \mathbb{C}, |\alpha| = 1\}$.

We now show how the machinery of this section leads to the same result. To determine $\mathscr{K}_+$, we must find the solutions of $T^*\psi = i\psi$. If $\psi \in D(T^*)$, then $\psi \in AC[0, 1]$, and the equality $i\, d\psi/dx = i\psi$ shows that ψ' is also absolutely continuous. Repeating this argument shows that any solution of $T^*\psi = i\psi$ is in fact infinitely differentiable and satisfies $\psi' = \psi$. Thus $\mathscr{K}_+ = \{ce^x | c \in \mathbb{C}\}$, and similarly $\mathscr{K}_- = \{ce^{-x} | c \in \mathbb{C}\}$. Therefore, the deficiency indices of T are $\langle 1, 1\rangle$. Let

$$\varphi_+ = \frac{\sqrt{2}}{\sqrt{e^2 - 1}} e^x \qquad \text{and} \qquad \varphi_- = \frac{\sqrt{2}\, e}{\sqrt{e^2 - 1}} e^{-x}$$

be normalized vectors from $\mathscr{K}_\pm$. Then the only partial isometries of $\mathscr{K}_+$ into $\mathscr{K}_-$ are the maps $\varphi_+ \mapsto \gamma\varphi_-$ where $|\gamma| = 1$. By Theorem X.2, the only symmetric extensions of T are the operators $A_\gamma = i\, d/dx$ with domain

$$D(A_\gamma) = \{\varphi + \beta\varphi_+ + \gamma\beta\varphi_- \,|\, \varphi \in D(T), \beta \in \mathbb{C}\}$$

By the last statement of Theorem X.2, each A_γ has zero deficiency indices and is therefore self-adjoint. To see that these are the same operators we got before, notice that if $\psi \in D(A_\gamma)$, then

$$\psi(0) = \frac{\beta(1 + \gamma e)\sqrt{2}}{\sqrt{e^2 - 1}} \qquad \text{and} \qquad \psi(1) = \frac{\sqrt{2}\,\beta(\gamma + e)}{\sqrt{e^2 - 1}}$$

so

$$\psi(1) = \frac{\gamma + e}{1 + \gamma e}\psi(0) = \alpha\psi(0) \qquad \text{where} \quad |\alpha| = \left|\frac{\gamma + e}{1 + \gamma e}\right| = 1$$

Conversely, if $\psi(1) = \alpha\psi(0)$, then ψ can be written $\psi = \varphi + \beta\varphi_+ + \gamma\beta\varphi_-$ for some β where $\gamma = (\alpha - e)/(1 - \alpha e)$. Thus, $A_\gamma = T_\alpha$.

We now examine the same problem from a "physical" point of view. Suppose that we have a smooth wave packet $\varphi(x)$ on $[0, 1]$ which is zero near the end points and which is being translated to the right (Figure X.1). For small enough y (so that the packet does not get to the end), the translations are given by the family of operators $U(y)$: $\varphi(x) \to \varphi(x - y)$. In quantum mechanics, translation should be represented by a unitary group whose generator is the momentum operator. For the wave packet $\varphi(x)$, this is the case:

$$\lim_{y \to 0} \frac{U(y)\varphi - \varphi}{iy} = \lim_{y \to 0} \frac{\varphi(x - y) - \varphi(x)}{iy} = i\frac{d}{dx}\varphi$$

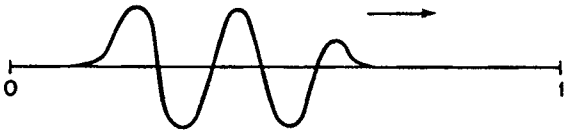


FIGURE X.1 The wave packet $\varphi(x)$.

So, the generator of translation acts like $i\,d/dx$ on the functions with support away from the end points. In fact, $i\,d/dx$ is symmetric on $C_0^1(0, 1)$, the C^1 functions of compact support on (0, 1), and its closure is just our operator T. But T is not self-adjoint and the reason is clear: We have specified the translation $U(y)$ only for functions whose support does not contain zero or one and then only for sufficiently small y (depending on the support). We must specify what happens when the wave packet gets to the end! If we want translation to be represented by a unitary group, then what goes out at one end must come in at the other (as though the interval [0, 1] were bent into a circle). That is, unitarity requires

$$\int_0^1 |\varphi(x - y)|^2\,dx = \int_0^1 |\varphi(x)|^2\,dx$$

where $x - y$ means translation mod 1. However, we still have the freedom of choosing the phase of the wave packet as it comes in at zero. By the superposition principle all functions must change by the same phase when they come back in. Thus the different "translations" are just given by specifying α, $|\alpha| = 1$ and by requiring that all reasonable wave packets $\psi_y \equiv \varphi(\cdot + y)$ satisfy $\psi_y(1) = \alpha\psi_y(0)$ for *all* times y. This motion is just given by e^{iyT_α} where T_α is the operator described above. Thus, even in this physically trivial situation we see that *different* self-adjoint extensions correspond to *different physics.*

A simple and useful criterion for a symmetric operator to have self-adjoint extensions is given by the following theorem.

Definition An antilinear map $C: \mathscr{H} \to \mathscr{H}$ $(C(\alpha\varphi + \beta\psi) = \bar{\alpha}C\varphi + \bar{\beta}C\psi)$ is called a **conjugation** if it is norm-preserving and $C^2 = I$.

Theorem X.3 (von Neumann's theorem) Let A be a symmetric operator and suppose that there exists a conjugation C with $C: D(A) \to D(A)$ and $AC = CA$. Then A has equal deficiency indices and therefore has self-adjoint extensions.

Proof Since $C^2 = I$ and $CD(A) \subseteq D(A)$, we have $CD(A) = D(A)$. Suppose that $\varphi_+ \in \mathscr{K}_+$ and $\psi \in D(A)$. Then

$$\begin{aligned} 0 &= \overline{(\varphi_+, (A + i)\psi)} = (C\varphi_+, C(A + i)\psi) \\ &= (C\varphi_+, (A - i)C\psi) \end{aligned}$$

Since C takes $D(A)$ onto $D(A)$, $C\varphi_+ \in \mathscr{K}_-$, so $C: \mathscr{K}_+ \to \mathscr{K}_-$. A similar proof shows that $C: \mathscr{K}_- \to \mathscr{K}_+$. Since C preserves norms,

$$\dim[\mathscr{K}_+] = \dim[\mathscr{K}_-] \quad \blacksquare$$

Example 2 (Schrödinger particle on a half-line) Let A be the operator $-d^2/dx^2$ on $L^2(0, \infty)$ with domain $C_0^\infty(0, \infty)$. Since complex conjugation commutes with A, we immediately know from Theorem X.3 that the deficiency indices of A are equal. We want to find the solutions of $A^*\varphi = \pm i\varphi$. Since $L^2(0, \infty) \subset \mathscr{D}'_{(0,\infty)}$, we are just looking for weak solutions (see Section V.4) of $-d^2\varphi/dx^2 = \pm i\varphi$. It follows from the regularity theorem (Theorem IX.25) that these solutions are infinitely differentiable and thus strong solutions. By elementary ordinary differential equations the strong solutions of $-\varphi''(x) = +i\varphi(x)$ are

$$\exp((-1 + i)x/\sqrt{2}), \qquad \exp((1 - i)x/\sqrt{2})$$

and the strong solutions of $-\varphi''(x) = -i\varphi(x)$ are $\exp((1 + i)x/\sqrt{2})$, $\exp((-1 - i)x/\sqrt{2})$. Since only $\exp((-1 + i)x/\sqrt{2})$ and $\exp((-1 - i)x/\sqrt{2})$ are in $L^2(0, \infty)$, we see that the deficiency indices are $\langle 1, 1\rangle$. Using Theorem X.2 and an analysis similar to the second part of Example 1, the reader can easily show (Problem 5) that the self-adjoint extensions of A can be parametrized by $\mathbb{R} \cup \{\infty\}$ with

$$D(A_a) = \{\psi \,|\, \psi \in AC^2[0, \infty], \psi'(0) + a\psi(0) = 0\}$$

if $a \in \mathbb{R}$ and

$$D(A_\infty) = \{\psi \,|\, \psi \in AC^2[0, \infty], \psi(0) = 0\}$$

The extensions all act on their respective domains by $-d^2/dx^2$. $AC^2[0, 1]$ is just the set of functions in $L^2[0, 1]$ whose weak derivatives are in $AC[0, 1]$, in particular, they are continuously differentiable.

The physical interpretation of these boundary conditions is as follows. Since the momentum operator is $i^{-1}\, d/dx$ and $i^{-1}\,(d/dx)e^{-ikx} = -ke^{-ikx}$, the function e^{-ikx} is a plane wave moving to the left with momentum

$k > 0$, i.e. an incoming wave of momentum k. e^{ikx} is an outgoing wave of momentum k. Let $a < \infty$ be fixed. The functions e^{ikx} and e^{-ikx} are not in $L^2(0, \infty)$ because of their behavior at ∞, but we ignore that since we are interested in behavior around the origin. Neither e^{ikx} or e^{-ikx} is in $D(A_a)$ near zero since they do not satisfy the boundary conditions. But if $\alpha = (ik - a)/(ik + a)$, then $e^{-ikx} + \alpha e^{ikx}$ satisfies the boundary conditions $\psi'(0) + a\psi(0)$ and is in $D(A_a)$ (ignoring the behavior at ∞). Thus the operator A_a generates the dynamics in which a plane wave of momentum k is reflected at the origin with the change of phase $\alpha(k) = (ik - a)/(ik + a)$. The case $a = \infty$ corresponds to a hard wall potential where the phase change for all momenta is $\alpha = -1$. Notice that the phase change for various plane waves is different for the different self-adjoint extensions. Thus, the *different* self-adjoint extensions correspond to *different* physics.

A less trivial application of Theorem X.3 is used in the following example in which only the *existence* of some self-adjoint extension is needed. The reader should compare this example to the similar proof of Bochner's theorem (Theorem IX.9) where the corresponding existence statement was derived from Stone's theorem.

Example 3 (the Hamburger moment problem) Let ρ be a positive measure on $\mathbb{R}$ and define

$$a_n = \int_{-\infty}^{\infty} x^n \, d\rho(x) \tag{X.8}$$

The numbers a_n are called the **moments** of the measure ρ. The Hamburger moment problem is to determine conditions on a sequence of real number $\{a_n\}_{n=0}^{\infty}$, so that there exists a measure satisfying (X.8). There is a very elegant solution.

Theorem X.4 A sequence of real numbers $\{a_n\}$ are the moments of a positive measure on $\mathbb{R}$ if and only if for all N and all $\beta_0, \ldots, \beta_N \in \mathbb{C}$,

$$\sum_{n,m=0}^{N} \bar{\beta}_n \beta_m a_{n+m} \geq 0 \tag{X.9}$$

Proof Suppose first that ρ is a positive measure and (X.8) holds. Then

$$\sum_{n,m=0}^{N} \bar{\beta}_n \beta_m a_{n+m} = \int_{-\infty}^{\infty} \left| \sum_{n=0}^{N} \beta_n x^n \right|^2 d\rho \geq 0$$

Conversely, suppose that (X.9) holds. Let P denote the set of polynomials on $\mathbb{R}$ with complex coefficients and define a sesquilinear form on P by

$$\left(\sum_{n=0}^{N} \beta_n x^n, \sum_{m=0}^{M} \alpha_m x^m\right) = \sum_{n=0}^{N} \sum_{m=0}^{M} \bar{\beta}_n \alpha_m a_{n+m}$$

By (X.9) the form is nonnegative. Let $Q = \{\psi \mid \psi \in P, (\psi, \psi) = 0\}$ and let $\mathscr{H}$ be the Hilbert space obtained by completing P/Q in the inner product $(\cdot, \cdot)$. Consider the map $A: P \to P$ defined by

$$A: \sum_{n=0}^{N} \beta_n x^n \to \sum_{n=0}^{N} \beta_n x^{n+1}$$

It is not hard to see that A is symmetric and $A: Q \to Q$ since the Schwarz inequality implies that

$$(A\psi, A\psi) = |(A^2\psi, \psi)| \leq (A^2\psi, A^2\psi)^{1/2}(\psi, \psi)^{1/2}$$

Thus, A lifts to a symmetric operator $\hat{A}$ on $\mathscr{H}$ with domain P/Q. If C denotes the usual complex conjugation on P, then C also lifts to a map $\hat{C}: P/Q \to P/Q$. It is easily checked that $\hat{C}$ extends to a conjugation on $\mathscr{H}$ and $\hat{A}\hat{C} = \hat{C}\hat{A}$. By Theorem X.3, $\hat{A}$ has some self-adjoint extension, call it $\tilde{A}$. Let ρ be the spectral measure for the vector 1 in P. Then

$$\int x^n \, d\rho(x) = (1, \tilde{A}^n 1) = (1, x^n) = a_n \quad \blacksquare$$

In Chapter XVI we will see that the Hahn–Banach theorem can be used to provide another proof of Theorem X.4. In Section X.6, we discuss the uniqueness aspects of the Hamburger moment problem.

Appendix to X.1 Motion on a half-line, limit point–limit circle methods

Any blockhead can cite generalities, but the mastermind discerns the particular cases they represent. *George Eliot in* ***Daniel Deronda***

In this appendix, we discuss both the classical motion and the quantum-mechanical motion of a particle in a potential on a half-line. Comparing these two cases brings out nicely both the analogies and the differences between classical and quantum mechanics and provides an opportunity to apply the theorems on deficiency indices to derive the limit point–limit

circle theory of ordinary differential equations. Furthermore, information about quantum-mechanical problems on a half-line can be used to analyze spherically symmetric multidimensional problems (see Example 4).

We begin with the classical case. Let $x(t)$ and $v(t)$ be the position and velocity of a particle moving on the half-line $(0, \infty)$ in a potential $V(x)$ which we assume has a continuous derivative $V'(x)$ which is Lipschitz uniformly on every compact subset of $(0, \infty)$. The Hamiltonian for the system is $H(x, v) = \frac{1}{2}mv^2 + V(x)$ and the equations of motion are

$$\dot{x}(t) = v(t), \qquad \dot{v}(t) = \frac{-1}{m} V'(x(t)) \tag{X.10}$$

For each given $x_0 > 0$, v_0, $t_0 > 0$, the standard contraction mapping argument (see Section V.6) gives the existence of a unique solution pair $\langle x(t), v(t)\rangle$ for t near t_0 satisfying $x(t_0) = x_0$, $v(t_0) = v_0$. The following proposition shows that the only case where a local solution does not extend to a global solution is when the particle runs into zero or off to infinity in finite time.

Proposition 1 Suppose that a global solution of (X.10) satisfying $x(t_0) = x_0 > 0$, $v(t_0) = v_0$ does not exist, that is, the maximal interval on which the solution with the initial conditions exists is $[t_0, \tau)$ where $\tau < \infty$. Then either

$$\lim_{t \uparrow \tau} x(t) = 0 \qquad \text{or} \qquad \lim_{t \uparrow \tau} x(t) = \infty$$

Proof By the construction of local solutions in Section V.6, and the assumptions made above on $V(x)$, for any compact subset K of $(0, \infty) \times \mathbb{R}$, there is a T_K so that (X.10) has a unique solution for $t \in (t_1 - T_K, t_1 + T_K)$ with specified values $\langle x_1, v_1\rangle \in K$ at $t = t_1$. From this we see that if the solution cannot be extended past $t = \tau$, then it cannot lie in K for any $t > \tau - T_K$. To complete the proof we must strengthen this statement that the point $\langle x(t), v(t)\rangle$ must eventually leave any compact subset of the phase space $(0, \infty) \times \mathbb{R}$ to the statement that $x(t)$ eventually leaves any compact subset C of $(0, \infty)$. It is here that conservation of energy enters critically. Since $H(x(t), v(t)) = H(x_0, v_0) = E_0$, if $x(t)$ lies in some compact subset C, then $\langle x(t), v(t)\rangle$ is contained in the compact set

$$C \times \left\{ v(t) \,\middle|\, |v(t)| \leq \sqrt{\frac{2}{m}} \left(E_0 - \inf_{x \in C} V(x) \right)^{1/2} \right\}$$

Thus for each n there is a t_n so that $x(t) \notin (1/n, n)$ for $t > t_n$ which by the continuity of $x(t)$ proves the proposition. ∎

The above argument shows how conservation of energy may be used to prove global existence for a classical system of one degree of freedom. In Section X.13 we will use the same energy conservation method to prove global existence for a classical system with an infinite number of degrees of freedom.

Definition We say that the classical motion generated by V is **complete** at 0 (respectively at ∞) if there is no $\langle x_0, v_0 \rangle \in (0, \infty) \times \mathbb{R}$ so that the solution $x(t)$ runs off to 0 (respectively to ∞) in a finite time.

Thus if V is complete at both 0 and ∞, global solutions exist for all initial conditions $\langle x_0, v_0 \rangle$. The following theorem settles the question of when V is complete.

Theorem X.5 Let $V(x)$ have a continuous derivative which is uniformly Lipschitz on each compact subset of $(0, \infty)$. Then the classical motion generated by $V(x)$:

(a) is not complete at 0 if and only if $V(x)$ is bounded above near zero;
(b) is not complete at ∞ if and only if V is bounded above for $x \geq 1$ and

$$\int_1^\infty \frac{dx}{\sqrt{K - V(x)}} < \infty \qquad \text{for some } K > \sup_{x \geq 1} V(x)$$

Proof V is not bounded above at zero if and only if there is a sequence $x_n \to 0$ so that $V(x_n) \to \infty$. Suppose V is not bounded above at zero. By conservation of energy

$$\tfrac{1}{2}mv(t)^2 + V(x(t)) = \tfrac{1}{2}mv_0^2 + V(x_0)$$

so $V(x(t)) \leq \frac{1}{2}mv_0^2 + V(x_0)$. Thus $x(t)$ can never equal x_n for n sufficiently large and so $x(t)$ can never get near zero. Thus V is complete at zero. Conversely, suppose $V(x) \leq M$ on $(0, 1)$. Let $x(0) = x_0 = 1$ and choose v_0 negative and so that $\frac{1}{2}mv_0^2 + V(1) = 1 + M$. Then $\frac{1}{2}mv(t)^2 \geq 1$ for all t so the particle gets to zero in a finite time. This proves (a).

If $V(x)$ is not bounded above on $(1, \infty)$, then the same argument as above shows that V is complete at ∞. So, suppose that $V(x) \leq M$ for $x \in [1, \infty)$, and that for some initial conditions $\langle x_0, v_0 \rangle$ and a $\tau < \infty$, $\tau \in \mathbb{R}$ we have $\lim_{t \to \tau} x(t) = \infty$. Let $K = \max\{M + 1, \frac{1}{2}mv_0^2 + V(x_0)\}$. Then, for all $t \in (0, \tau)$,

$$\left| \frac{dx}{dt} \right| \leq \sqrt{\frac{2}{m}} \sqrt{K - V(x(t))}$$

Once the motion starts going to the right, $x(t)$ must be strictly increasing because if it were not, conservation of energy and the uniqueness of solutions of (X.10) imply that it would never get to ∞. Thus there is a $t_1 < \tau$ so that $t \in (t_1, \tau)$ implies $dx/dt > 0$ and $x(t) \geq 1$. Therefore

$$\sqrt{\frac{m}{2}} \int_{x(t_1)}^{\infty} \frac{dx}{\sqrt{K - V(x)}} \leq \int_{x(t_1)}^{\infty} \frac{dt}{dx}\, dx = \tau - t_1 < \infty$$

Conversely, if

$$\int_1^{\infty} \frac{dx}{\sqrt{K - V(x)}} < \infty \qquad \text{for some } K > \sup_{x \geq 1} V(x)$$

we choose initial conditions $x_0 = 1$, $v_0 > 0$, so that $E = \frac{1}{2}mv_0^2 + V(x_0) = K$. Then $dx/dt > 0$ for all $t > 0$ and

$$\int_0^{\infty} \left(\frac{dt}{dx}\right) dx = \sqrt{\frac{m}{2}} \int_1^{\infty} \frac{dx}{\sqrt{K - V(x)}} < \infty$$

so the travel time to ∞ is finite. ∎

We turn now to the quantum-mechanical case where we need only assume that $V(x)$ is a real-valued, continuous function on $(0, \infty)$. The quantum analogue of the classical Hamiltonian $H(x, v)$ is the formal operator $-(2m)^{-1}\, d^2/dx^2 + V(x)$. We will denote by H the operator $-d^2/dx^2 + V(x)$ on $L^2(0, \infty)$ with domain $D(H) = C_0^{\infty}(0, \infty)$, the C^{∞} functions with support away from 0 and ∞ (we drop the inessential $1/2m$). Using the fact that $V(x)$ is real-valued and a simple integration by parts, we see that H is a symmetric operator. Suppose that $\psi \in D(H^*)$, then

$$\left(-\frac{d^2}{dx^2}\varphi + V\varphi, \psi\right) = (\varphi, H^*\psi)$$

or

$$\left(-\frac{d^2}{dx^2}\varphi, \psi\right) = (\varphi, H^*\psi) - (\varphi, V\psi)$$

for all $\varphi \in C_0^{\infty}(0, \infty)$. Thus the second weak derivative of ψ is locally L^2 since $V(x)\psi(x)$ is locally L^2. By Sobolev's lemma, ψ' is absolutely continuous and $-\psi'' - V\psi \in L^2(0, \infty)$ (although each of the separate terms may not be in L^2 near zero or infinity). Therefore, the functions in $D(H^*)$ are quite nice and the action of H^* is just what we expect. Finally, we note that H commutes with complex conjugation so its deficiency indices are equal. We summarize in a proposition.

Proposition 2 Suppose $V(x)$ is a real valued continuous function on $(0, \infty)$ and let H be the operator $-d^2/dx^2 + V(x)$ with domain $C_0^\infty(0, \infty)$. Then

(a) H is symmetric.
(b) If $\psi \in D(H^*)$, then ψ is continuously differentiable, ψ' is absolutely continuous, ψ'' is locally L^2, $-\psi'' + V\psi \in L^2(0, \infty)$, and

$$H^*\psi = -\psi'' + V\psi$$

(c) H has equal deficiency indices.

The importance of Proposition 2 is that it shows that questions about the deficiency indices of H reduce to questions about the classical ordinary differential equations $-\psi'' + V\psi = \pm i\psi$. We prepare for our analysis with:

Proposition 3 Let $Q(x)$ be a continuous complex-valued function on $(0, \infty)$. Then the set of solutions of $\varphi''(x) = Q(x)\varphi(x)$ on $(0, \infty)$ is a two-dimensional vector space of twice continuously differentiable functions. For any two solutions φ and ψ, the **Wronskian** $W(x) = \varphi'(x)\psi(x) - \varphi(x)\psi'(x)$ is constant and equals zero if and only if φ and ψ are linearly dependent as functions.

Proof We will prove the existence of a global solution with arbitrarily specified data $\langle \varphi(1), \varphi'(1) \rangle \in \mathbb{C}^2$ at $x = 1$. By the discussion in Section V.6, local solutions exist, so as in the proof of Proposition 1, a global solution can fail to exist only if $\alpha(x) = \langle \varphi(x), \varphi'(x) \rangle$ goes to infinity at some finite $x_\circ$ different from zero. We will show that this cannot happen for any $x_\circ > 1$; the proof for $x_\circ < 1$ is similar. Define

$$q(x_\circ) = \sup\{|Q(x)| + 1 \mid 1 \le x \le x_\circ\}$$

Then, from the differential equation we have

$$\alpha'(x) = \langle \varphi'(x), Q(x)\varphi(x) \rangle$$

for $1 \le x \le x_\circ$, so

$$|\alpha'(x)| \le q(x_\circ)|\alpha(x)|$$

and

$$|\alpha(x)| \le |\alpha(1)| + q(x_\circ) \int_1^x |\alpha(y)|\, dy \tag{X.11}$$

Thus, by iterating (X.11),

$$|\alpha(x)| \leq |\alpha(1)| e^{q(x_0)(x-1)}$$

for $1 \leq x \leq x_0$. This proves the existence of at least two independent global solutions. Furthermore, by local uniqueness there are at most two, so there are exactly two.

The statements about $W(x)$ follow immediately by differentiation and by observing that $W(x)$ is the determinant of

$$\begin{pmatrix} \psi & \varphi \\ \psi' & \varphi' \end{pmatrix} \blacksquare$$

We now investigate the deficiency indices of H by studying the solutions of

$$-\varphi''(x) + V(x)\varphi(x) = \lambda\varphi(x) \tag{X.12}$$

Theorem X.6 Let $V(x)$ be a continuous real-valued function on $(0, \infty)$.

(a) If $\operatorname{Im} \lambda \neq 0$, then at least one nonzero solution of (X.12) is in L^2 near zero and at least one solution is in L^2 near ∞.

(b) If for one $\lambda \in \mathbb{C}$, both solutions of (X.12) are in L^2 near infinity (respectively near zero) then, for *all* $\lambda \in \mathbb{C}$, both solutions of (X.12) are in L^2 near infinity (respectively near zero).

Proof Consider first the operator B on $L^2(1, 2)$ with domain $D(B) = \{u \in AC^2[1, 2] \mid u(1) = u(2) = u'(1) = u'(2) = 0\}$ and with $Bu = -u'' + Vu$. By mimicking the arguments used in Examples 1 and 2 of Section X.1 and by using Proposition 3, one finds that B has deficiency indices $\langle 2, 2\rangle$. In particular, if $\operatorname{Im} \lambda \neq 0$, $\operatorname{Ran}(B - \lambda)$ is not dense in $L^2(1, 2)$. We can thus find $v \in C_0^\infty(1, 2)$ with $v \notin \operatorname{Ran}(B - \lambda)$.

Now, let $\tilde{H}$ be a self-adjoint extension of the operator H on $L^2(0, \infty)$. Since $\operatorname{Im} \lambda \neq 0$, we can find $u \in D(\tilde{H}) \subset D(H^*)$ satisfying $(\tilde{H} - \lambda)u = v$. It is impossible that u vanish identically on both $(0, 1)$ and $(2, \infty)$, for if it did, its restriction to $[1, 2]$ would lie in $D(B)$ thereby contradicting the condition that $v \notin \operatorname{Ran}(B - \lambda)$.

Suppose that u does not vanish identically on $(0, 1)$. Then the restriction $\tilde{u}$ of u to $(0, 1)$ satisfies (X.12) on $(0, 1)$ and is square integrable near 0. Let $D(A) = \{f \in D(\tilde{H}) \mid f \equiv 0 \text{ in } [1, \infty)\}$, viewed as a (dense) subset of $L^2(0, 1)$. The operator $A - \lambda \equiv (\tilde{H} - \lambda) \restriction D(A)$ does not have dense range since $\bar{\tilde{u}}$, the complex conjugate of $\tilde{u}$, obeys: $\bar{\tilde{u}} \in D(A^*)$ and $(A^* - \bar{\lambda})\bar{\tilde{u}} = 0$. As a result, we can find $w \in C_0^\infty(0, 1)$ with $w \notin \operatorname{Ran}(A - \lambda)$. Since $\tilde{H}$ is self-adjoint, we can find $f \in D(\tilde{H})$ with $(\tilde{H} - \lambda)f = w$. Since $w \notin \operatorname{Ran}(A - \lambda)$,

f cannot vanish identically in $[1, \infty)$ and we thereby obtain a nonzero solution of (X.12) square integrable near ∞. If u does not vanish identically on $(2, \infty)$, a similar argument can be used. This proves (a).

To prove (b), let us suppose that φ_1 and φ_2 are two independent solutions of (X.12) for some $\lambda_0 \in \mathbb{C}$ and that both φ_1 and φ_2 are L^2 near ∞, and are normalized so that $\varphi_1'(x)\varphi_2(x) - \varphi_1(x)\varphi_2'(x) = 1$. Let u be a solution of (X.12) for $\lambda = \lambda_1 \neq \lambda_0$. Choose $c \in (0, \infty)$. Then an explicit computation shows that

$$u(x) - (\lambda_1 - \lambda_0)\int_c^x (\varphi_1(x)\varphi_2(\xi) - \varphi_1(\xi)\varphi_2(x))u(\xi)\, d\xi$$

satisfies (X.12) with $\lambda = \lambda_0$, so

$$u(x) = c_1\varphi_1(x) + c_2\varphi_2(x) + (\lambda_1 - \lambda_0)\int_c^x (\varphi_1(x)\varphi_2(\xi) - \varphi_1(\xi)\varphi_2(x))u(\xi)\, d\xi$$

for some constants c_1 and c_2. Define $\|f\|_{[c,x]}^2 = \int_c^x |f(x)|^2\, dx$ and choose M so that $\|\varphi_1\|_{[c,\infty]} < M$ and $\|\varphi_2\|_{[c,\infty]} < M$. Then, by the Schwarz inequality,

$$|u(x)| \leq |c_1||\varphi_1(x)| + |c_2||\varphi_2(x)| + |\lambda_1 - \lambda_0|(|\varphi_1(x)| + |\varphi_2(x)|)M\|u\|_{[c,x]}$$

so

$$\|u\|_{[c,x]} \leq |c_1|M + |c_2|M + 2M^2|\lambda_1 - \lambda_0|\|u\|_{[c,x]}$$

Thus if $|\lambda_1 - \lambda_0| \leq 1/4M^2$, $\frac{1}{2}\|u\|_{[c,x]} \leq (|c_1| + |c_2|)M$ for all x, so u is in L^2 near ∞. Since we can choose M as small as we like by choosing c large, we have proven (b) for the case at infinity. The case at zero is proved similarly. ∎

We will say that $V(x)$ is in the **limit circle case** at infinity (respectively at zero) if for some, and therefore all, λ, *all* solutions of

$$-\varphi''(x) + V(x)\varphi(x) = \lambda\varphi(x)$$

are square integrable at infinity (respectively at zero). If $V(x)$ is not in the limit circle case at infinity (respectively at zero), it is said to be in the **limit point case**. For the origin of this terminology, see the Notes. We can now prove:

Theorem X.7 (Weyl's limit point–limit circle criterion) Let $V(x)$ be a continuous real-valued function $(0, \infty)$. Then $H = -d^2/dx^2 + V(x)$ is essentially self-adjoint on $C_0^\infty(0, \infty)$ if and only if $V(x)$ is in the limit point case at both zero and infinity.

Proof If $V(x)$ is in the limit circle case at both zero and infinity, then the deficiency indices of H are $\langle 2, 2\rangle$. If $V(x)$ is limit circle at one end and limit point at the other, then H has deficiency indices $\langle 1, 1\rangle$. So if $V(x)$ is not limit point at both ends, then H is not essentially self-adjoint.

Now, suppose that $V(x)$ is limit point at both ends. For $f, g \in D(H^*)$, we set $W_x(f, g) = \overline{f(x)}g'(x) - \overline{f'(x)}g(x)$. W_x is continuous and

$$W_b(f, g) - W_a(f, g) = \int_a^b [\overline{(H^*f)(x)}g(x) - \overline{f(x)}(H^*g)(x)]\, dx$$

by integration by parts. Since the integrand on the right-hand side is in $L^1(0, \infty)$, the limits $W_\infty(f, g) = \lim_{b\to\infty} W_b(f, g)$ and $W_0(f, g) = \lim_{a\to 0} W_a(f, g)$ exist and

$$W_\infty(f, g) - W_0(f, g) = (H^*f, g) - (f, H^*g)$$

If we can show that the left-hand side is zero, then H^* is symmetric and therefore H is essentially self-adjoint.

Choose $c \in (0, \infty)$. Let B be the restriction of H to $C_0^\infty(0, c) \subset L^2(0, c)$ and let A be $-d^2/dx^2 + V(x)$ on

$$D(A) = \{\varphi \mid \varphi \in C^\infty(0, c),\ \varphi = 0 \text{ near zero},\ \varphi(c) = 0\}$$

Since $B \subset A$, we have $\overline{B} \subset \overline{A}$. But there are functions in $D(\overline{A})$ with $\varphi'(c) \neq 0$ and no such functions are in $D(\overline{B})$ so $\overline{A}$ is a *proper* closed symmetric extension of $\overline{B}$. Since both solutions of $-\varphi'' + V\varphi = \pm i\varphi$ are L^2 near c, but only one is L^2 near zero, the deficiency indices of B are $\langle 1, 1\rangle$. Therefore, the deficiency indices of $\overline{A}$ are $\langle 0, 0\rangle$, so $\overline{A}$ is self-adjoint.

Now, let $f, g \in D(H^*)$ and choose $f_1, g_1 \in C_0^\infty(0, \infty)$ be such that $f(c) + f_1(c) = 0$, $g(c) + g_1(c) = 0$. Set $f_2 = f + f_1$, $g_2 = g + g_1$. Then

$$\begin{aligned} -W_0(f, g) &= W_c(f_2, g_2) - W_0(f_2, g_2) \\ &= (\overline{A}f_2, g_2) - (f_2, \overline{A}g_2) = 0 \end{aligned}$$

since $f_2, g_2 \in D(A^*) = D(\overline{A})$. Thus, $W_0(f, g) = 0$ and a similar proof shows that $W_\infty(f, g) = 0$. ∎

We now want to investigate when $V(x)$ is in the limit point case at both ends. The discussion in Examples 1 and 2 of Section 1 suggests that H will be essentially self-adjoint if and only if in the classical motion generated by $V(x)$ the particle stays away from 0 and ∞ so that we need not specify boundary conditions at zero or infinity (we will see presently to what extent this classical-quantum analogy holds). We define:

Definition The potential $V(x)$ is called **quantum-mechanically complete** if $H = -d^2/dx^2 + V(x)$ is essentially self-adjoint on $C_0^\infty(0, \infty)$. $V(x)$ is said to be **complete at** ∞ (respectively **at 0**) if at least one solution of $\varphi''(x) = V(x)\varphi(x)$ is not in L^2 near ∞ (respectively near 0).

In Example 2 of Section 1 we showed that the potential $V(x) \equiv 0$ is not complete. This is not surprising since a classical particle in a zero potential which starts out moving to the left will get to zero in finite time.

First we discuss the case at ∞. The standard sufficient condition is:

Theorem X.8 Let $V(x)$ be a continuous real-valued function on $(0, \infty)$ and suppose that there exists a positive differentiable function $M(x)$ so that

(i) $V(x) \geq -M(x)$

(ii) $\int_1^\infty (M(x))^{-1/2}\, dx = \infty$

(iii) $M'(x)/(M(x))^{3/2}$ is bounded near ∞.

Then $V(x)$ is in the limit point case (complete) at ∞.

Proof We will show that both solutions of $-\varphi'' + V\varphi = 0$ cannot be in L^2 near ∞. If $0 < c_1 < c < \infty$ and u is a real solution in L^2 near ∞, then

$$-K_1 \equiv -\int_{c_1}^\infty u^2(x)\, dx \leq -\int_{c_1}^c u^2(x)\, dx \leq \int_{c_1}^c \frac{V(x)}{M(x)}\, u^2(x)\, dx$$

$$= \int_{c_1}^c \frac{u''(x)u(x)}{M(x)}\, dx$$

An integration by parts then proves that u satisfies

$$-\frac{u'(x)u(x)}{M(x)}\Bigg]_{c_1}^c + \int_{c_1}^c \frac{(u'(x))^2}{M(x)}\, dx - \int_{c_1}^c \frac{u'(x)u(x)M'(x)\, dx}{(M(x))^2} \leq K_1 \quad \text{(X.13)}$$

for all c. Using hypothesis (iii) we can find K_2 so that

$$\int_{c_1}^c \frac{u'(x)u(x)M'(x)}{(M(x))^2}\, dx \leq K_2 \left(\int_{c_1}^c \frac{(u'(x))^2}{M(x)}\, dx\right)^{1/2} \left(\int_{c_1}^c (u(x))^2\, dx\right)^{1/2}$$

Suppose that $\int_{c_1}^\infty ((u'(x)^2/M(x))\, dx = \infty$. Then by the last inequality, the hypothesis on u, and (X.13), $u'(x)u(x)$ is positive near ∞. But, this would imply that $u'(x)$ and $u(x)$ always have the same sign, which is impossible because since u is in L^2 near infinity. Thus, $\int_{c_1}^\infty ((u'(x)^2/M(x))\, dx < \infty$.

Now suppose that φ and ψ are independent solutions of $-\varphi'' + V\varphi = 0$ which are in L^2 near infinity. We may assume that φ and ψ are real-valued and that they are normalized so that $\varphi(x)\psi'(x) - \varphi'(x)\psi(x) = 1$. Then,

$$\left(\frac{1}{M(x)}\right)^{1/2} = \frac{\varphi(x)\psi'(x)}{(M(x))^{1/2}} - \frac{\varphi'(x)\psi(x)}{(M(x))^{1/2}}$$

would be in L^1 near infinity which contradicts hypothesis (ii). ∎

Corollary Let $V(x)$ be differentiable on $(0, \infty)$ and bounded above by K on $[1, \infty)$. Suppose that

(i) $\displaystyle\int_1^\infty \frac{dx}{\sqrt{K - V(x)}} = \infty.$

(ii) $V'(x)|V(x)|^{-3/2}$ is bounded near infinity.

Then $V(x)$ is in the limit point case at ∞.

Thus if $V(x)$ is classically complete at ∞ (condition (i)) and in addition satisfies condition (ii), then $V(x)$ is quantum-mechanically complete. Condition (ii) says essentially that the derivative of V should not be too large compared to V. The following two examples show that on physical as well as mathematical grounds the classical and quantum problems will not be equivalent if the derivative of V is too large.

Example 1 (V is quantum-mechanically complete but classically incomplete at ∞) The potential $V(x)$ will be a series of steps smoothly connected on very short intervals (α_i, β_i) (see Figure X.2). It is clear that $\int_0^\infty (1/\sqrt{-V(x)})\,dx < \infty$, so the classical motion is incomplete at ∞. We will show that if the steps are sharp enough, the quantum motion is complete at infinity. The physical reason for this behavior is that part of the quantum-mechanical wave is reflected at each of the sharp steps and the steps are arranged so that the reflected waves are coherent. To see the idea of the proof, consider the case of infinitely sharp steps when $\alpha_k = k = \beta_k$. Let $\varphi(x) = -\cos(n^2\pi x - \frac{1}{2}n(n-1)\pi)$ for $n - 1 \le x \le n$. Then $\varphi \in D(H^*)$, $\varphi'' = V\varphi$, and $\varphi \notin L^2$ near infinity. We now show that we can smooth out this infinitely sharp step potential so that one solution of

$$\varphi''(x) = V(x)\varphi(x) \tag{X.14}$$

remains not in $L^2(0, \infty)$.

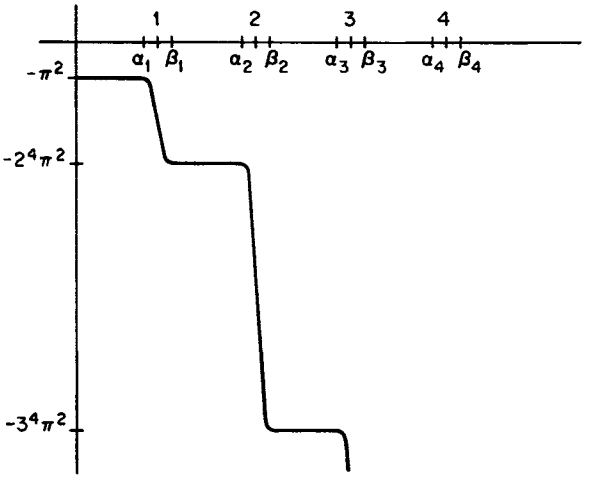


FIGURE X.2 The graph of V.

On the short intervals (α_k, β_k), V will be monotone decreasing in such a way that V is twice continuously differentiable. We take $\alpha_1 = 1$ and let $\varphi(x) = -\cos(\pi x)$ on $(0, 1]$. At $x = 1$, $\varphi(1) = 1$ and $\varphi'(1) = 0$. We want to pick β_1 so that the solution has not descended much at β_1. Since $V(x) < 0$, the solution will be concave downward until the next zero of $\varphi(x)$, call it r_1. On the interval $I_1 = (1, \min\{r_1, \alpha_2\})$, $\varphi(x)$ satisfies

$$\varphi(x) - 1 = \int_1^x \left(\int_1^s V(t)\varphi(t)\, dt \right) ds \tag{X.15}$$

which implies that

$$|\varphi(x) - 1| \leq \frac{(x-1)^2}{2} \left(\sup_{I_1} |V(t)| \right) \left(\sup_{I_1} |\varphi(t)| \right)$$

$$\leq \frac{(x-1)^2}{2} (2^4\pi^2)$$

We choose β_1 so that $|\varphi(\beta_1) - 1| \leq \frac{1}{4}$. Now we can put in the potential on the interval (α_1, β_1): the point is that whichever smooth connection we choose, the above a priori estimate guarantees that $\varphi(\beta_1) \geq 1 - \frac{1}{4}$. On (β_1, α_2), $\varphi(x)$ has the form $\varphi_2(x) = A_2 \cos(2^2\pi x - \gamma_2)$ where $|A_2| \geq 1 - \frac{1}{4}$. Now, choose α_2 to be the closest point to $x = 2$ where φ_2 has a maximum. We choose β_2 (using the same idea as above) so that $\varphi(\beta_2) \geq 1 - \frac{1}{4} - \frac{1}{8}$.

We proceed in this way to construct a solution $\varphi(x)$ which is

$$A_n \cos(n^2\pi x - \gamma_n)$$

on (β_{n-1}, α_n) with $|A_n| \geq \frac{1}{2}$. Thus $\varphi \notin L^2(0, \infty)$ so by Theorem X.6, V is in the limit point case at ∞.

Example 2 (V is classically complete but quantum-mechanically incomplete at ∞) Our potential will be of the form

$$V(x) = \frac{1}{x^2} - x^4 + \sum_{k=1}^{\infty} \sigma_k(x)$$

where the σ_k are very narrow smooth spikes of increasing height so that $V(k) = k$ (see Figure X.3). Since V is not bounded from above at ∞, the motion is classically complete. It follows from Theorem X.9 (below) that the potential $V_1(x) = x^{-2} - x^4$ is not quantum-mechanically complete at ∞, so that the corresponding Hamiltonian H_1 is not essentially self-adjoint on $C_0^\infty(0, \infty)$. We will use a perturbation method from Section X.2 to show that $H = H_1 + \sum \sigma_k(x)$ is similarly not essentially self-adjoint on $C_0^\infty(0, \infty)$ if the spikes σ_k are narrow enough. Since the potential $V = V_1 + \sum \sigma_k$ is limit point at zero by Theorem X.10 (below), it must be limit circle at infinity. The physical reason for this behavior is that if the spikes are narrow enough, the quantum particle can tunnel through them even though the classical particle is turned back.

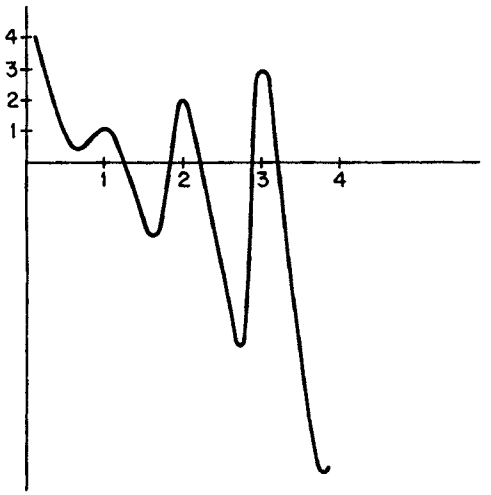


FIGURE X.3 The graph of V.

To prove that H is not essentially self-adjoint, we will show that, in the language of Section X.2, $\sum \sigma_k$ is $(-d^2/dx^2 + V_1)$-bounded with bound less than one on $C_0^\infty(0, \infty)$. That is, for some $a < 1$,

$$\|(\textstyle\sum \sigma_k)\varphi\|^2 \leq a^2\|-\varphi'' + V_1\varphi\|^2 + b^2\|\varphi\|^2 \tag{X.16}$$

for all $\varphi \in C_0^\infty(0, \infty)$. By the symmetric form of the Kato–Rellich theorem (Theorem X.13), this implies that $-d^2/dx^2 + V_1$ and $-d^2/dx^2 + V_1 + \sum \sigma_k$ are either both essentially self-adjoint or both not essentially self-adjoint on $C_0^\infty(0, \infty)$.

To prove (X.16) we use the following Sobolev-type estimate which the reader is asked to prove in Problem 10. Let $x_0 \in \mathbb{R}$, $\varphi \in C_0^\infty(\mathbb{R})$, and let $I_4^y = \{x \mid |x - y| \leq \frac{1}{4}\}$ and $I_2^y = \{x \mid |x - y| \leq \frac{1}{2}\}$. Then there is a constant C, independent of φ and y, so that

$$\sup_{x \in I_4^y} |\varphi|^2 \leq C(\|\varphi''\|^2_{L^2(I_2^y)} + \|\varphi\|^2_{L^2(I_2^y)}) \tag{X.17}$$

Let $\sigma_k(x) \in C_0^2(I_4^k)$ be such that $V_1(x) + \sigma_k(x)$ reaches its maximum in I_4^k at k and the value at the maximum is k. Let $\varepsilon(k)$ denote the diameter of the support of $\sigma_k(x)$. Then for $\varphi \in C_0^\infty(\mathbb{R})$,

$$\begin{aligned}\|\sigma_k\varphi\|^2 &\leq 4\varepsilon(k)k^8 \sup_{I_4^k} |\varphi|^2 \\ &\leq 4\varepsilon(k)k^8(\|\varphi''\|^2_{L^2(I_2^k)} + \|\varphi\|^2_{L^2(I_2^k)}) \\ &\leq 8\varepsilon(k)k^8[\|-\varphi'' + V_1\varphi\|^2_{L^2(I_2^k)} + \|V_1\varphi\|^2_{L^2(I_2^k)} + \|\varphi\|^2_{L^2(I_2^k)}]\end{aligned}$$

since $\|\psi_1\|^2 \leq \|\psi_1\|^2 + \|\psi_1 + 2\psi_2\|^2 = 2\|\psi_1 + \psi_2\|^2 + 2\|\psi_2\|^2$. Now, choose $\varepsilon(k)$ so small that $8\varepsilon(k)k^8 \leq \frac{1}{2}$ and $\sup_{x \in I_2^k} |16\varepsilon(k)k^8 V_1(x)| \leq 1$. Then

$$\begin{aligned}\left\| \sum_{k=1}^{\infty} \sigma_k \varphi \right\|^2 &= \sum_{k=1}^{\infty} \|\sigma_k \varphi\|^2 \\ &\leq \sum_{k=1}^{\infty} (\tfrac{1}{2}\|-\varphi'' + V_1\varphi\|^2_{L^2(I_2^k)} + 2\|\varphi\|^2_{L^2(I_2^k)}) \\ &\leq \tfrac{1}{2}\|-\varphi_1'' + V_1\varphi\|^2 + 2\|\varphi\|^2\end{aligned}$$

This completes the proof of (X.16).

The following theorem shows that if the derivatives of V are not too large compared to V itself, then V is classically complete at ∞ if and only if it is quantum-mechanically complete at ∞ (for the proof, see the references in the Notes).

Theorem X.9 Let V be a twice continuously differentiable real-valued function on $(0, \infty)$ and suppose that $V(x) \to -\infty$ as $x \to \infty$. Suppose further that

$$\int_c^\infty \left(\frac{[(-V)^{1/2}]'}{(-V)^{3/2}} \right)' (-V)^{-1/4}\, dx < \infty$$

for some c. Then V is in the limit point case at ∞ if and only if $\int_c^\infty (-V(x))^{-1/2}\, dx = \infty$, i.e., if and only if V is classically complete at ∞.

Example 3 Let $c > 0$. One easily concludes from this theorem that $-d^2/dx^2 - cx^\alpha$ is in the limit point case at ∞ if and only if $\alpha \leq 2$. For further discussion of this example, see Section X.5.

We turn now to the question of completeness at zero. There is a wide variety of theorems which guarantee either the limit point or limit circle case at zero. The following theorem gives conditions for positive potentials.

Theorem X.10 Let V be continuous and *positive* near zero. If $V(x) \geq \frac{3}{4}x^{-2}$ near zero then $-d^2/dx^2 + V(x)$ is in the limit point case at zero. If for some $\varepsilon > 0$, $V(x) \leq (\frac{3}{4} - \varepsilon)x^{-2}$ near zero, then $-d^2/dx^2 + V(x)$ is in the limit circle case.

Proof We deal first with the case where $V(x) = c/x^2$, $c > 0$. Two independent solutions of the equation $-\varphi''(x) + (c/x^2)\varphi(x) = 0$ are x^{α_1} and x^{α_2} where $\alpha_1 = (1 + \sqrt{1 + 4c})/2$ and $\alpha_2 = (1 - \sqrt{1 + 4c})/2$. x^{α_1} is always in L^2 near zero but x^{α_2} is in L^2 near zero if and only if $\alpha_2 > -\frac{1}{2}$, i.e., if and only if $c < \frac{3}{4}$. Thus $-\varphi''(x) + (c/x^2)\varphi(x) = 0$ has two independent solutions in L^2 near zero if and only if $c < \frac{3}{4}$.

We now prove the theorem by a comparison argument. Suppose that V and $\tilde{V}$ are both positive on an interval $(0, b)$ and $V(x) \geq \tilde{V}(x)$. Suppose $A > 0$ and let u_A be a solution of $u''(x) = V(x)u(x)$ satisfying $u(b/2) = 2$, $u'(b/2) = -A$, and let $\tilde{u}_A$ be a solution of $u''(x) = \tilde{V}(x)u(x)$ satisfying $\tilde{u}(b/2) = 1$, $\tilde{u}'(b/2) = -A/2$. A short argument shows that $u_A(x) > \tilde{u}_A(x)$ for all $x \in (0, b/2)$. Choosing A to be two different positive numbers we get two independent solutions of the two equations respectively. This shows that if $\tilde{u}''(x) = \tilde{V}(x)\tilde{u}(x)$ has a solution which is not L^2 near zero, then so does $u''(x) = V(x)u(x)$. Thus, if $-d^2/dx^2 + \tilde{V}(x)$ is limit point near zero, then so

is $-d^2/dx^2 + V(x)$, and if $-d^2/dx^2 + V(x)$ is limit circle, then so is $-d^2/dx^2 + \tilde{V}(x)$. Combining these statements with the results when $V(x) = cx^{-2}$ proves the theorem. ∎

Another useful condition is that $-d^2/dx^2 + V(x)$ is limit circle at zero if $V(x)$ is decreasing as x goes to zero. The proof is outlined in Problem 7. As in the case at ∞ (Example 2), it is possible to construct a potential V so that V is classically incomplete at zero but quantum-mechanically complete.

The following example shows that information about problems on a half-line can be used in certain multidimensional problems.

Example 4 (spherically symmetric potentials) A potential on $\mathbb{R}^n$ which only depends on $r = (\sum_{i=1}^n x_i^2)^{1/2}$, the distance from the origin, is called spherically symmetric. Let $D = C_0^\infty(\mathbb{R}^n\backslash\{0\})$, the C^∞ functions with compact support away from the origin. We will investigate $-\Delta + V(r)$ on D. We may regard each $\varphi \in L^2(\mathbb{R}^n)$ as a function of r and $n-1$ variables ξ on the sphere S^{n-1}. In terms of these variables

$$\|f\|_2^2 = \int_0^\infty \left(\int_{S^{n-1}} |f(r, \xi)|^2 \, d\Omega \right) r^{n-1} \, dr$$

where $d\Omega$ is the usual area measure on the sphere. Let $\tilde{D}$ be the set of functions in D which are finite linear combinations of products $f(r)g(\xi)$. $\tilde{D}$ is also dense in $L^2(\mathbb{R}^n)$ by Theorem II.10 since $L^2(\mathbb{R}^n) = L^2(\mathbb{R}^+, r^{n-1}\,dr) \otimes L^2(S^{n-1}, d\Omega)$. On functions of the form $f(r)g(\xi)$, $-\Delta + V(r)$ acts by

$$(-\Delta + V(r))f(r)g(\xi) = \left(-\frac{d^2}{dr^2} + V(r) - \frac{n-1}{r}\frac{d}{dr} \right) f(r)g(\xi) - \frac{1}{r^2} f(r)Bg(\xi)$$

where B is the Laplace–Beltrami operator on $L^2(S^{n-1})$. It turns out (see the Notes) that B is essentially self-adjoint and negative on $C^\infty(S^{n-1})$, has only point spectrum of finite multiplicity, and that the corresponding eigenfunctions are C^∞. We will denote by K_ℓ the eigenspace corresponding to the ℓth eigenvalue κ_ℓ (we list the eigenvalues in decreasing order starting with $\kappa_0 = 0$). Then

$$L^2(\mathbb{R}^+, r^{n-1}\,dr) \otimes L^2(S^{n-1}, d\Omega) = \bigoplus_{\ell=0}^{\infty} L_\ell$$

where

$$L_\ell = L^2(\mathbb{R}^+, r^{n-1}\,dr) \otimes K_\ell$$

Define $D_\ell = \tilde{D} \cap L_\ell$, then

$$(-\Delta + V(r)) \restriction D_\ell = \left(-\frac{d^2}{dr^2} - \frac{n-1}{r}\frac{d}{dr} + V(r) - \frac{\kappa_\ell}{r^2} \right) \otimes I$$

By Theorem VIII.33 and Problem 1a, to conclude that $-\Delta + V(r)$ is essentially self-adjoint on $\tilde{D}$ and therefore on D, we need only prove that for each ℓ,

$$-\frac{d^2}{dr^2} - \left(\frac{n-1}{r}\right)\frac{d}{dr} + V(r) - \frac{\kappa_\ell}{r^2}$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^+) \subset L^2(\mathbb{R}^+, r^{n-1}\,dr)$.

Let $U\colon L^2(\mathbb{R}^+, r^{n-1}\,dr) \to L^2(\mathbb{R}^+, dr)$ be the unitary operator $U\colon \varphi(r) \mapsto r^{(n-1)/2}\varphi(r)$. U takes $C_0^\infty(\mathbb{R}^+)$ into itself and

$$U\left(-\frac{d^2}{dr^2} - \frac{n-1}{r}\frac{d}{dr} + V(r) - \frac{\kappa_\ell}{r^2} \right) U^{-1}$$

$$= -\frac{d^2}{dr^2} + V(r) + \left(\frac{(n-1)(n-3)}{4} - \kappa_\ell \right)\frac{1}{r^2} \tag{X.18a}$$

Each κ_ℓ is less than or equal to zero, so by Theorem X.10, each of these operators will be essentially self-adjoint on $C_0^\infty(\mathbb{R}^+)$ if

$$V(r) + \frac{(n-1)(n-3)}{4}\frac{1}{r^2} \geq \frac{3}{4r^2} \tag{X.18b}$$

On the other hand, if

$$0 \leq V(r) + \frac{(n-1)(n-3)}{4}\frac{1}{r^2} \leq \frac{c}{r^2}, \qquad c < \frac{3}{4} \tag{X.18c}$$

then one or more of the operators in (X.18a) will not be essentially self-adjoint on $C_0^\infty(\mathbb{R}^+)$. Thus, we have proven the following theorem:

Theorem X.11 Let $V(r)$ be a continuous symmetric potential on $\mathbb{R}^n\backslash\{0\}$. If $V(r)$ satisfies (X.18b), then $-\Delta + V(r)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n\backslash\{0\})$. If $V(r)$ satisfies (X.18c), then $-\Delta + V(r)$ is not essentially self-adjoint on $C_0^\infty(\mathbb{R}^n\backslash\{0\})$.

We remark that this theorem shows in particular that $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n\backslash\{0\})$ if and only if $n \geq 4$. This fact is somewhat subtle if $n = 4$ but can be more easily proven if $n \geq 5$ (Problem 9). The first half of Theorem X.11 has a generalization to the noncentral case; see Section X.4.

X.2 Perturbations of self-adjoint operators

In this section we will prove several theorems which say that if A is self-adjoint and B is not too large compared to A, then $A + B$ is self-adjoint. These theorems have fundamental applications in quantum mechanics. First we define what we mean by a "small" perturbation.

Definition Let A and B be densely defined linear operators on a Hilbert space $\mathscr{H}$. Suppose that:

(i) $D(B) \supset D(A)$
(ii) For some a and b in $\mathbb{R}$ and all $\varphi \in D(A)$,

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\| \tag{X.19a}$$

Then B is said to be **A-bounded**. The infimum of such a is called the **relative bound** of B with respect to A. If the relative bound is zero, we say that B is **infinitesimally small** with respect to A and write $B << A$. We remark that usually b must be chosen larger as a is chosen smaller.

Sometimes, it is convenient to replace (ii) in the above definition by

(iii) For some $\tilde{a}, \tilde{b} \in \mathbb{R}$ and all $\varphi \in D(A)$,

$$\|B\varphi\|^2 \leq \tilde{a}^2\|A\varphi\|^2 + \tilde{b}^2\|\varphi\|^2 \tag{X.19b}$$

If (iii) holds, then (ii) holds with $a = \tilde{a}$, $b = \tilde{b}$. And if (ii) holds, we can conclude that (iii) holds with $\tilde{a}^2 = (1 + \varepsilon)a^2$, $\tilde{b}^2 = (1 + \varepsilon^{-1})b^2$ for each $\varepsilon > 0$. Thus, the infimum over all a in (ii) is equal to the infimum over all $\tilde{a}$ in (iii). Note that to prove estimates of the form (ii) or (iii) it is sufficient to prove them on a core for A.

A fundamental perturbation result is:

Theorem X.12 (the Kato–Rellich theorem) Suppose that A is self-adjoint, B is symmetric, and B is A-bounded with relative bound $a < 1$. Then $A + B$ is self-adjoint on $D(A)$ and essentially self-adjoint on any core of A. Further, if A is bounded below by M, then $A + B$ is bounded below by $M - \max\{b/(1 - a), a|M| + b\}$ where a and b are given by (X.19a).

Proof We will show that $\mathrm{Ran}(A + B \pm i\mu_0) = \mathscr{H}$ for some $\mu_0 > 0$. For $\varphi \in D(A)$, we have

$$\|(A + i\mu)\varphi\|^2 = \|A\varphi\|^2 + \mu^2\|\varphi\|^2$$

Letting $\varphi = (A + i\mu)^{-1}\psi$, we conclude from this that $\|A(A + i\mu)^{-1}\| \leq 1$ and $\|(A + i\mu)^{-1}\| \leq \mu^{-1}$. Therefore, applying (X.19a) with $\varphi = (A + i\mu)^{-1}\psi$, we find that

$$\begin{aligned}\|B(A + i\mu)^{-1}\psi\| &\leq a\|A(A + i\mu)^{-1}\psi\| + b\|(A + i\mu)^{-1}\psi\| \\ &\leq \left(a + \frac{b}{\mu}\right)\|\psi\|\end{aligned}$$

Thus, for μ_0 large, $C = B(A + i\mu_0)^{-1}$ has norm less than one, since $a < 1$. This implies that $-1 \notin \sigma(C)$, so $\mathrm{Ran}(I + C) = \mathscr{H}$. Since A is self-adjoint, $\mathrm{Ran}(A + i\mu_0) = \mathscr{H}$ also. Thus the equation

$$(I + C)(A + i\mu_0)\varphi = (A + B + i\mu_0)\varphi \qquad \text{for} \quad \varphi \in D(A)$$

implies that $\mathrm{Ran}(A + B + i\mu_0) = \mathscr{H}$. The proof that $\mathrm{Ran}(A + B - i\mu_0) = \mathscr{H}$ is the same. Thus, by the fundamental criterion (Theorem VIII.3), $A + B$ is self-adjoint on $D(A)$.

It is a direct consequence of (X.19) that $D(\overline{(A + B) \upharpoonright D_0}) \supset D(\overline{A \upharpoonright D_0})$, so $A + B$ is essentially self-adjoint on any core of A.

Finally we prove the semiboundedness statement. Suppose that $t \in \mathbb{R}$ and $-t < M$. Then $\mathrm{Ran}(A + t) = \mathscr{H}$ and the same estimates as before show that $\|B(A + t)^{-1}\| < 1$ if

$$-t < M - \max\left\{\frac{b}{1 - a}, a|M| + b\right\}$$

Thus for such t, $\mathrm{Ran}(A + B + t) = \mathscr{H}$ and $(A + B + t)^{-1} = (A + t)^{-1} \times (I + C)^{-1}$ which implies that $-t \in \rho(A + B)$. ∎

The following symmetric form of the Kato–Rellich theorem is sometimes useful. For an application, see Example 3 in the Appendix to Section X.1.

Theorem X.13 Let A and C be symmetric operators. Suppose that D is a linear subspace satisfying $D \subseteq D(A)$, $D \subseteq D(C)$, and that

$$\|(A - C)\varphi\| \leq a(\|A\varphi\| + \|C\varphi\|) + b\|\varphi\|$$

for all $\varphi \in D$, where $a < 1$. Then,

(a) A is essentially self-adjoint on D if and only if C is essentially self-adjoint on D.

(b) $D(\overline{A \upharpoonright D}) = D(\overline{C \upharpoonright D})$.

Proof Let $B = A - C$ with $D(B) = D$ and define $F(\alpha) = C + \alpha B$ for $0 \le \alpha \le 1$. Then $F(0) = C$, $F(1) = A$ and $C\varphi = F(\alpha)\varphi - \alpha B\varphi$, $A\varphi = F(\alpha)\varphi + (1 - \alpha)B\varphi$ for all $\varphi \in D$. Thus, the inequality in the hypothesis implies that

$$\begin{aligned}\|B\varphi\| &\le a(\|A\varphi\| + \|C\varphi\|) + b\|\varphi\| \\ &\le 2a\|F(\alpha)\varphi\| + a\|B\varphi\| + b\|\varphi\|\end{aligned}$$

or

$$\|B\varphi\| \le \frac{2a}{1-a}\|F(\alpha)\varphi\| + \frac{b}{1-a}\|\varphi\| \tag{X.20}$$

Let $0 \le \alpha' \le 1$. If $2a\alpha'/(1 - a) < 1$, (X.20) and Theorem X.12 imply that $F(\alpha + \alpha') = F(\alpha) + \alpha' B$ is essentially self-adjoint on D if and only if $F(\alpha)$ is. Thus, starting with $\alpha = 0$ and applying this result finitely many times, we conclude (a). The reader is asked (Problem 13) to follow similar steps to prove (b). ∎

The following theorem extends Theorem X.12 to the case of relative bound one, but it has a slightly weaker conclusion.

Theorem X.14 (Wüst's theorem) Let A be self-adjoint and B be symmetric with $D(B) \supset D(A)$. Suppose that for some b and all $\varphi \in D(A)$,

$$\|B\varphi\| \le \|A\varphi\| + b\|\varphi\| \tag{X.21a}$$

Then $A + B$ is *essentially* self-adjoint on $D(A)$ or any core for A.

Proof By a simple argument, it is enough to show that $A + B$ is essentially self-adjoint on $D(A)$. Suppose that $(A + B + i)^* h = 0$. For each $t < 1$, $A + tB$ is self-adjoint on $D(A)$ by Theorem X.12. Thus, there exists $\varphi_t \in D(A)$ with $\|\varphi_t\| \le \|h\|$, so that $(A + tB + i)\varphi_t = h$. Define $\psi_t = h - (t - 1)B\varphi_t$. Then a short calculation shows that $(\psi_t, h) = 0$. By (X.21a),

$$\begin{aligned}\|A\varphi_t\| &\le \|(A + tB)\varphi_t\| + \|tB\varphi_t\| \\ &\le \|(A + tB)\varphi_t\| + t\|A\varphi_t\| + tb\|\varphi_t\|\end{aligned}$$

so

$$(1 - t)\|A\varphi_t\| \le \|(A + tB)\varphi_t\| + tb\|\varphi_t\|$$

Since $\|(A + tB)\varphi_t\|^2 = \|h\|^2 - \|\varphi_t\|^2$, this implies that $(1 - t)\|A\varphi_t\|$ is bounded as $t \uparrow 1$. It follows by using (X.21a) again that $(1 - t)\|B\varphi_t\|$ and therefore also $\|\psi_t\|$ are bounded as $t \uparrow 1$. Now let $\eta \in D(A)$. Then

$$\lim_{t \uparrow 1}(\psi_t - h, \eta) = \lim_{t \uparrow 1}(t - 1)(\varphi_t, B\eta) = 0$$

Since the $\|\psi_t\|$ are uniformly bounded, we conclude that $h = w-\lim \psi_t$. But then $(h, h) = \lim(h, \psi_t) = 0$ so $h = 0$. We conclude that $\mathrm{Ker}(A + B + i)^* = \{0\}$. The proof that $\mathrm{Ker}(A + B - i)^* = \{0\}$ is similar. ∎

Choosing $A = -B$ shows that "essentially self-adjoint" cannot be replaced by "self-adjoint" in the statement of Theorem X.14. We also note that there are counterexamples which show that the conclusion of the theorem may be false if the relative bound is larger than one. (See Example 4 at the end of this section.) We also note that according to our discussion of (X.19a) and (X.19b), the condition (X.21a) needed to apply Theorem X.14 is itself implied by the condition

$$\|B\varphi\|^2 \leq \|A\varphi\|^2 + b^2\|\varphi\|^2 \tag{X.21b}$$

which is equivalent to the operator inequality

$$B^2 \leq A^2 + b^2 \tag{X.21c}$$

We come now to Kato's basic application of the Kato–Rellich theorem to atomic Hamiltonians. First, we define some new classes of functions.

Definition Let $\langle M, \mu\rangle$ be a measure space. The set of measurable functions f on M which can be written $f = f_1 + f_2$ where $f_1 \in L^2(M, d\mu)$ and $f_2 \in L^\infty(M, d\mu)$ will be denoted by $L^2(M, d\mu) + L^\infty(M, d\mu)$.

Theorem X.15 Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ be real-valued. Then $-\Delta + V(x)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ and self-adjoint on $D(-\Delta)$.

Proof Since V is real-valued, the operator of multiplication by V is self-adjoint on

$$D(V) = \{\varphi \,|\, \varphi \in L^2(\mathbb{R}^3),\ V\varphi \in L^2(\mathbb{R}^3)\}$$

Let $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. Then

$$\|V\varphi\|_2 \leq \|V_1\|_2 \|\varphi\|_\infty + \|V_2\|_\infty \|\varphi\|_2 \tag{X.22}$$

so $D(V) \supset C_0^\infty(\mathbb{R}^3)$. By Theorem IX.28, given any $a > 0$, there is a $b > 0$ so that

$$\|\varphi\|_\infty \leq a\|\Delta\varphi\|_2 + b\|\varphi\|_2 \tag{X.23}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. This inequality and (X.22) give

$$\|V\varphi\|_2 \leq a\|V_1\|_2 \|-\Delta\varphi\|_2 + (b + \|V_2\|_\infty)\|\varphi\|_2$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. Thus V is $-\Delta$-bounded with arbitrarily small bound on $C_0^\infty(\mathbb{R}^3)$. Since $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$, the Kato–Rellich theorem implies that $-\Delta + V$ is also essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. ∎

Example 1 Let $V(r) = -e^2/r$ where $r = \sqrt{x^2 + y^2 + z^2}$. Then $-\Delta - e^2/r$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$.

Theorem X.16 (Kato's theorem) Let $\{V_k\}_{k=1}^m$ be a collection of real-valued measurable functions each of which is in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Let $V_k(\mathbf{y}_k)$ be the multiplication operator on $L^2(\mathbb{R}^{3n})$ obtained by choosing $\mathbf{y}_k$ to be three coordinates of $\mathbb{R}^{3n}$. Then $-\Delta + \sum_{k=1}^m V_k(\mathbf{y}_k)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3n})$, where Δ denotes the Laplacian on $\mathbb{R}^{3n}$.

Proof First we consider one of the functions V_k separately. By a rotation of variables we may assume the variables in $V_k(\cdot)$ are x_1, x_2, x_3. (This is because $\|\cdot\|_2$, $\|\cdot\|_\infty$, and $-\Delta$ are invariant under rotations of coordinates.) Let Δ_1 denote the Laplacian with respect to x_1, x_2, x_3. By the estimate (X.23), together with the "equivalence" of the bounds (X.19a) and (X.19b), we have for all $\varphi \in C_0^\infty(\mathbb{R}^{3n})$,

$$\begin{aligned}
\|V_k\varphi\|^2_{L^2(\mathbb{R}^{3n})} &\le a^2 \int |-\Delta_1 \varphi(x_1, \ldots, x_{3n})|^2 \, dx_1 \cdots dx_{3n} \\
&\quad + b^2 \int |\varphi(x_1, \ldots, x_{3n})|^2 \, dx_1 \cdots dx_{3n} \\
&= a^2 \int \left| \sum_{i=1}^3 p_i^2 \hat{\varphi}(p_1, \ldots, p_{3n}) \right|^2 dp_1 \cdots dp_{3n} + b^2 \|\varphi\|^2 \\
&\le a^2 \int \left| \sum_{i=1}^n p_i^2 \hat{\varphi}(p_1, \ldots, p_{3n}) \right|^2 dp_1 \cdots dp_{3n} + b^2 \|\varphi\|^2 \\
&= a^2 \|-\Delta\varphi\|^2 + b^2 \|\varphi\|^2
\end{aligned}$$

Thus, using the Schwarz inequality, one easily concludes that

$$\left\| \sum_{k=1}^m V_k(\mathbf{y}_k)\varphi \right\|^2 \le m^2 a^2 \|-\Delta\varphi\|^2 + m^2 b^2 \|\varphi\|^2$$

for all $\varphi \in C_0^\infty(\mathbb{R}^{3n})$. Since a may be chosen as small as we like, we conclude that $\sum_{k=1}^m V_k(\mathbf{y}_k)$ is infinitesimally small with respect to $-\Delta$. Thus, by the Kato–Rellich theorem, $-\Delta + \sum_{k=1}^m V_k(\mathbf{y}_k)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. ∎

Example 2 (atomic Hamiltonians) Let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ in $\mathbb{R}^3$ be orthogonal coordinates for $\mathbb{R}^{3n}$. Then

$$-\sum_{i=1}^{n} \Delta_i - \sum_{i=1}^{n} \frac{ne^2}{|\mathbf{x}_i|} + \sum_{i<j}^{n} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3n})$.

For an application of the Kato–Rellich theorem to ordinary differential operators, see Problem 7.

There is a form analogue of the Kato–Rellich theorem which can be used when the form $(B\varphi, \varphi)$ is "small" with respect to the form $(A\varphi, \varphi)$ even though B may not be A-bounded. Although the statement of the theorem below is similar to Theorem X.12, the proof is very different.

Theorem X.17 (the KLMN theorem) Let A be a positive self-adjoint operator and suppose that $\beta(\varphi, \psi)$ is a symmetric quadratic form on $Q(A)$ such that

$$|\beta(\varphi, \varphi)| \leq a(\varphi, A\varphi) + b(\varphi, \varphi) \qquad \text{all } \varphi \in D(A) \tag{X.24}$$

for some $a < 1$ and $b \in \mathbb{R}$. Then there exists a unique self-adjoint operator C with $Q(C) = Q(A)$ and

$$(\varphi, C\psi) = (\varphi, A\psi) + \beta(\varphi, \psi) \qquad \text{all } \varphi, \psi \in Q(C)$$

C is bounded below by $-b$ and any domain of essential self-adjointness for A is a form core for C.

Proof Define a form $\gamma(\varphi, \psi) = (\varphi, A\psi) + \beta(\varphi, \psi)$ on $Q(A)$. By (X.24),

$$\begin{aligned} \gamma(\varphi, \varphi) &\geq (1 - a)(\varphi, A\varphi) - b(\varphi, \varphi) \\ &\geq -b(\varphi, \varphi) \end{aligned}$$

since A is positive. Thus γ is bounded from below by $-b$. Furthermore

$$\begin{aligned} (1 - a)(\varphi, A\varphi) + (\varphi, \varphi) &\leq \gamma(\varphi, \varphi) + (b + 1)(\varphi, \varphi) \\ &\leq (1 + a)(\varphi, A\varphi) + (2b + 1)(\varphi, \varphi) \end{aligned}$$

Thus the $\|\cdot\|_{+1,A}$ and $\|\cdot\|_{+1,\gamma}$ norms are equivalent on $Q(A)$. Since $Q(A)$ is closed under $\|\cdot\|_{+1,A}$, it is closed under $\|\cdot\|_{+1,\gamma}$. Thus γ is a semi-bounded, closed quadratic form on $Q(A)$. The theorem now follows from the statement and proof of Theorem VIII.15. ∎

This theorem suggests that we define:

Definition Let A be a positive self-adjoint operator. Suppose that B is a self-adjoint operator which satisfies:

(i) $Q(B) \supset Q(A)$
(ii) $|(\varphi, B\varphi)| \leq a(\varphi, A\varphi) + b(\varphi, \varphi), \varphi \in Q(A)$

for some $a > 0$ and $b \in \mathbb{R}$. Then B is said to be **relatively form-bounded** with respect to A. If a can be chosen arbitrarily small, B is said to be **infinitesimally form-bounded** with respect to A (written $B \prec\prec A$).

If B is self-adjoint and relatively form-bounded ($a < 1$) with respect to a positive self-adjoint operator A, then the KLMN theorem gives meaning to $A + B$. We emphasize that this definition of "$A + B$" may *differ* from the operator sum. There are examples where B is relatively form-bounded with respect to A even though $D(A) \cap D(B) = \{0\}$. In fact, as the following example shows, the form β in the KLMN theorem need not be a form arising from an operator or even a closable form.

Example 3 Let $A = -d^2/dx^2$ on $\mathbb{R}$ and define $\beta(\varphi, \psi) = \overline{\varphi}(0)\psi(0)$ for $\varphi, \psi \in C_0^\infty(\mathbb{R})$. By Sobolev's lemma, for any $a > 0$, there is a b so that

$$\|\varphi\|_\infty^2 \leq a(\varphi, -\varphi'') + b\|\varphi\|^2$$

Thus we can apply the KLMN theorem to define $-d^2/dx^2 + \delta$! A function $\psi \in Q(-d^2/dx^2) \subset C_\infty(\mathbb{R})$ is in the domain of $-d^2/dx^2 + \delta$ if and only if $-\psi''(x) + \delta(x)\psi(0) \in L^2(\mathbb{R})$ where the derivative is taken in the sense of distributions. For example, if $\psi(x)$ looks like $1 + \frac{1}{2}|x|$ near zero and is C^∞ away from zero with compact support, then $\psi \in D(-d^2/dx^2 + \delta(x))$, since the $\delta(x)\psi(0)$ will just cancel the term $-\delta(x)\psi(x)$ which appears in $-\psi''(x)$. Thus, $D(A + B)$ can contain vectors which are neither in $D(A)$ nor in $D(B)$ but for which there are cancellations in "$A\psi + B\psi$."

The following theorem shows that if B is A-bounded, then B is form-bounded with respect to A.

Theorem X.18 Let A be a positive self-adjoint operator and suppose that B is self-adjoint. Then

(a) If B is A-bounded with relative bound a, then B is form-bounded with respect to A with relative bound a.
(b) $B << A$ implies $B \prec\prec A$.

Proof Let $C^\infty(A) = \bigcap_{n=1}^\infty D(A^n)$, $\mu > 0$, and let $\mathscr{H}_n$ be the closure of $C^\infty(A)$ under the norm $\|\varphi\|_n = \|(A + I)^{n/2}\varphi\|$, $n = 0, \pm 1, \pm 2, \ldots$. Then a map C from $C^\infty(A)$ to $\mathscr{H}$ extends to be a bounded operator from $\mathscr{H}_m$ to $\mathscr{H}_{-n}$ if and only if $(A + I)^{-n/2}C(A + I)^{-m/2}$ is bounded on $C^\infty(A)$ in the usual operator norm.

If B is A-bounded with relative bound a, then $B(A + \mu I)^{-1}$ and $(A + \mu I)^{-1}B$ are bounded by $(a + b/\mu)$. The interpolation argument in Example 3 of the Appendix to Section IX.4 proves that

$$(A + \mu I)^{-1/2}B(A + \mu I)^{-1/2}$$

is also bounded by $a + (b/\mu)$ and it follows immediately that

$$(\varphi, B\varphi) \leq \left(a + \frac{b}{\mu}\right)(\varphi, (A + \mu I)\varphi)$$

for $\varphi \in D_\infty(A)$. Since $\mu > 0$ is arbitrary, parts (a) and (b) follow. ∎

The KLMN theorem can sometimes be used to define Hamiltonians when Rellich's theorem does not apply. To see that the $L^2 + L^\infty$ class of potentials does not include all "reasonable" potentials, we remark that it is venerable physical folklore that potentials of the form $V_\alpha(r) = -r^{-\alpha}$ produce reasonable quantum dynamics as long as $\alpha < 2$. But $V_\alpha \in L^2 + L^\infty$ only if $\alpha < \frac{3}{2}$! Thus we cannot use Rellich's theorem if $\frac{3}{2} \leq \alpha < 2$ (see Problem 14). However, we can use the KLMN theorem. First, we prove an estimate:

Lemma (the uncertainty principle lemma) Let $\psi \in C_0^\infty(\mathbb{R}^3)$. Then

$$\int_{\mathbb{R}^3} \frac{1}{4r^2}\,|\psi(\mathbf{r})|^2\,d\mathbf{r} \leq \int_{\mathbb{R}^3} |\nabla\psi(\mathbf{r})|^2\,d\mathbf{r}$$

Proof We may suppose that ψ is real-valued. Then,

$$\nabla(r^{+1/2}\psi) = r^{1/2}\nabla\psi + \tfrac{1}{2}r^{-3/2}\mathbf{r}\psi$$

Thus, if $r \neq 0$,

$$\begin{aligned}
|\nabla\psi|^2 &= |r^{-1/2}\nabla(r^{1/2}\psi) - \tfrac{1}{2}r^{-2}\mathbf{r}\psi|^2 \\
&\geq -r^{-3/2}\psi\,\frac{\partial}{\partial r}(r^{1/2}\psi) + \frac{1}{4}\,r^{-2}|\psi|^2 \\
&= -\frac{1}{2r^2}\,\frac{\partial}{\partial r}(r|\psi|^2) + \frac{1}{4}\,r^{-2}|\psi|^2
\end{aligned}$$

So,

$$\int |\nabla\psi|^2\, d\mathbf{r} \geq \int \frac{1}{4r^2}\, |\psi|^2\, d\mathbf{r} - \frac{1}{2}\int_0^\infty \frac{\partial}{\partial r}\int_{S_2} r|\psi|^2\, d\Omega\, dr$$

$$= \int \frac{1}{4r^2}\, |\psi|^2\, d\mathbf{r} \quad \blacksquare$$

Proposition If $\alpha < 2$, then $-r^{-\alpha} \prec\prec -\Delta$.

Proof Let $\varphi \in C_0^\infty$ and let $a > 0$ be given. Choose $\varepsilon > 0$ so that $1/r^\alpha \leq a/4r^2$ for all $r \leq \varepsilon$. Then

$$\int_{\mathbb{R}^3} \frac{1}{r^\alpha}\, |\varphi(\mathbf{r})|^2\, d\mathbf{r} = \int_{|\mathbf{r}|\leq\varepsilon} \frac{1}{r^\alpha}\, |\varphi(\mathbf{r})|^2\, d\mathbf{r} + \int_{|\mathbf{r}|>\varepsilon} \frac{1}{r^\alpha}\, |\varphi(\mathbf{r})|^2\, d\mathbf{r}$$

$$\leq a\int_{|\mathbf{r}|\leq\varepsilon} |\nabla\varphi(\mathbf{r})|^2\, d\mathbf{r} + \frac{1}{\varepsilon^\alpha}\int_{|\mathbf{r}|>\varepsilon} |\varphi(\mathbf{r})|^2\, d\mathbf{r}$$

$$\leq a\int_{\mathbb{R}^3} (-\Delta\varphi(\mathbf{r}))\overline{\varphi(\mathbf{r})}\, d\mathbf{r} + \frac{1}{\varepsilon^\alpha}\int_{\mathbb{R}^3} |\varphi(\mathbf{r})|^2\, d\mathbf{r} \quad \blacksquare$$

This proposition shows that for $\frac{3}{2} \leq \alpha < 2$, we can use the KLMN theorem to define $-\Delta - r^{-\alpha}$. $L^2 + L^\infty$ is the natural class of potentials associated with the Kato–Rellich theorem (see Problem 14). There is no completely natural class associated with the KLMN theorem.

Definition A measurable function V on $\mathbb{R}^3$ is called a **Rollnik potential** if

$$\|V\|_R^2 \equiv \int_{\mathbb{R}^3} \frac{|V(x)|\,|V(y)|}{|x-y|^2}\, d^3x\, d^3y < \infty$$

We denote the set of Rollnik potentials by R.

R turns out to be a vector space which is complete under the Rollnik norm $\|\cdot\|_R$. Moreover, by Sobolev's inequality (IX.19), $L^{3/2}(\mathbb{R}^3) \subset R$; in particular $r^{-\alpha} \in R + L^\infty$ if $\alpha < 2$. The analogue of the Kato theorem is:

Theorem X.19

(a) If $V \in R + L^\infty(\mathbb{R}^3)$, then $V \prec\prec -\Delta$

(b) If $V_i(\mathbf{r})$ and $V_{ij}(\mathbf{r})$ are all in $R + L^\infty$ and

$$V = \sum V_i(\mathbf{r}_i) + \sum_{i,j=1}^{N} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

on $\mathbb{R}^{3N}$, then $V \prec\prec -\Delta$.

For the proof, see the references in the Notes or Problem 17. We remind the reader again that the meaning given to $-\Delta + V$ by the KLMN Theorem *may* differ from the operator sum defined on $D(-\Delta) \cap D(V)$.

The problem of determining conditions on a potential on $\mathbb{R}^s$ so that $-\Delta + V$ is essentially self-adjoint has been extensively studied using Rellich's theorem and the KLMN theorem. The proofs of the necessary inequalities often use the L^p-estimates of Section IX.4 and the interpolation theorems and therefore the results are usually dependent on the dimension s. We present two examples below. For other theorems, see Section X.4 and the references in the Notes.

Theorem X.20 Let $s \geq 4$. If $V \in L^p(\mathbb{R}^s)$ for some $p > s/2$, then $V << -\Delta$.

Proof By Theorem IX.27, we know that if $u \in D(-\Delta)$ then

$$(1 + k^2)\hat{u}(k) \in L^2(\mathbb{R}^s)$$

Further, since $p > s/2$, $(1 + k^2)^{-1} \in L^p(\mathbb{R}^s)$, so by the Hölder inequality $\hat{u} \in L^q$ and

$$\|\hat{u}\|_q \leq \|(1 + k^2)^{-1}\|_p \|(1 + k^2)\hat{u}\|_2$$

where $q^{-1} = p^{-1} + \frac{1}{2}$. Therefore, by the Hansdorff-Young inequality $u \in L^r(\mathbb{R}^s)$ where $r^{-1} = \frac{1}{2} - p^{-1}$. Since $V \in L^p$, it follows from the Hölder inequality that $Vu \in L^2$. Thus, $D(V) \supset D(-\Delta)$ and

$$\begin{aligned}\|Vu\|_2 \leq \|V\|_p \|u\|_r &\leq \|V\|_p \|\hat{u}\|_q \\ &= \|V\|_p \|(1 + tk^2)^{-1}(1 + tk^2)\hat{u}\|_q \\ &\leq \|V\|_p \|(1 + tk^2)^{-1}\|_p \|(1 + tk^2)\hat{u}\|_2 \\ &\leq (\|V\|_p \|(1 + k^2)^{-1}\|_p) t^{-s/2p} (\|u\|_2 + t\|-\Delta u\|_2)\end{aligned}$$

Since $p > s/2$. this estimate shows that $V << -\Delta$. ∎

The above theorem can be extended to the borderline case $p = s/2$ when $s \geq 5$, but in fact a stronger result is true.

Theorem X.21 (Strichartz's theorem) Let $s \geq 5$ and suppose $V \in L^{s/2}_w$. Then V is Δ-bounded with bound less than or equal to $C\|V\|_{s/2,w}$ where C depends only on s.

Proof It is sufficient to show that $\|V(I + \Delta)^{-1}\varphi\|_2 \leq C\|V\|_{s/2,w}\|\varphi\|_2$ for all $\varphi \in L^2(\mathbb{R}^s)$. Since $(I + \Delta)^{-1}\varphi = G * \varphi$ where G is the Fourier transform

of $(1 + p^2)^{-1}$ on $\mathbb{R}^s$, we need the properties of G established in Problems 49 *or* 50 of Chapter IX. Since $G(x)$ is exponentially decreasing at ∞ and $\overline{\lim}_{|x|\to 0} |x|^{s-2}|G(x)| < \infty$, we easily find that $\mu\{x \mid |G(x)| \geq t\}$ is bounded by $c_2 t^{s/s-2}$ for some $c_2 > 0$, where μ is Lebesgue measure. Thus, using the inequality in Problem 39 of Chapter IX, with $p = s/2$ and $q = 2$, we conclude that

$$\|V(G * \varphi)\|_2 \leq C_3 \|V\|_{s/2,\,w} \|G\|_{s/s-2,\,w} \|\varphi\|_2 \blacksquare$$

Corollary Let μ denote Lebesgue measure on $\mathbb{R}^s$, $s \geq 5$. If $V(x)$ is a real-valued measurable function and

$$\lim_{t\to\infty} t^{s/2}\mu\{x \mid |V(x)| \geq t\} = 0$$

then $V << -\Delta$. In particular, if $V \in L^{s/2}(\mathbb{R}^s)$, then $V << -\Delta$.

Example 4 Let $s = 5$. From Theorems X.10 and X.11, it follows that $-\Delta + \alpha/r^2$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^5\backslash\{0\})$ if and only if $\alpha \geq -1.25$. Further, $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^5\backslash\{0\})$. The reader can easily check that $1/r^2 \in L_w^{5/2}(\mathbb{R}^5)$, so by Strichartz' theorem, α/r^2 is $-\Delta$-bounded. Thus, the closure of $-\Delta + \alpha/r^2 \upharpoonright C_0^\infty(\mathbb{R}^5\backslash\{0\})$ contains

$$(-\Delta + \alpha/r^2) \upharpoonright C_0^\infty(\mathbb{R}^5)$$

Therefore, in the case $\alpha < -1.25$, $-\Delta + \alpha/r^2$ is not even essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$.

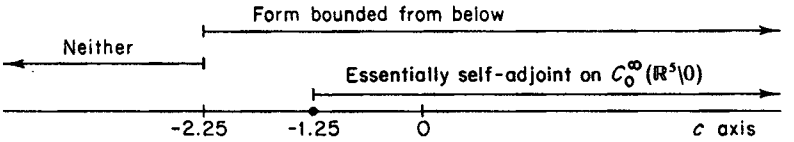


FIGURE X.4 The operator $-\Delta + (c/r^2)$ when $n = 5$.

In Problem 15, the reader is asked to show that $-d^2/dx^2 + c/x^2$ is form-bounded from below on $C_0^\infty(\mathbb{R}^+)$ if and only if $c \geq -\frac{1}{4}$. Thus, using the method of Example 4 of the Appendix to Section X.1, we conclude that $-\Delta + \alpha/r^2$ is form-bounded from below on $C_0^\infty(\mathbb{R}^5\backslash\{0\})$ if and only if $\alpha \geq -2.25$. Therefore, if α is in the range $-2.25 \leq \alpha < -1.25$, we can use the quadratic form techniques of Theorem VIII.15 to define $-\Delta + \alpha/r^2$, even though $-\Delta + \alpha/r^2$ is not essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$. See Figure X.4.

Example 5 (Schrödinger operators for systems with magnetic fields) According to the Lagrangian–Hamiltonian theory of classical mechanics, the energy operator written in terms of the coordinate $\mathbf{q}$ and the canonically conjugate momentum $\mathbf{p} = m\dot{\mathbf{q}} + e\mathbf{A}/c$ is

$$E = \frac{1}{2m}(\mathbf{p} - e\mathbf{A}/c)^2 + V(\mathbf{q})$$

where $\mathbf{A}$ is the **magnetic vector potential**, related to $\mathbf{B}$, the **magnetic field** by

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{X.25}$$

Using the correspondence between classical energy functions and quantum-mechanical Hamiltonian operators (Section VIII.11), we see that the Hamiltonian for an n-particle system in the presence of a magnetic field is

$$H = \sum_{j=1}^{n} (2m_j)^{-1}\left(-i\nabla_j - \frac{e_j}{c}\mathbf{A}\right)^2 + V(\mathbf{x}_1, \ldots, \mathbf{x}_n) \tag{X.26}$$

The case

$$A(\mathbf{x}) = \tfrac{1}{2}\mathbf{x} \times \mathbf{B}_0 \tag{X.27}$$

with $\mathbf{B}_0$ constant is especially important for this leads to $\mathbf{B} = \mathbf{B}_0$. This constant field situation is called the Zeeman effect, and its treatment requires special methods (see Section 4) since A grows at infinity. For the present, we note that perturbation methods do allow the treatment of some kinds of magnetic vector potentials. We give a detailed version of the operator perturbation theory result and leave the form result to the reader (Problem 36):

Theorem X.22 Suppose that each component of $\mathbf{A}$ is a real-valued function in $L^4(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, that $\nabla \cdot \mathbf{A} \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ (in the sense of distributions), and that V is a real-valued function in $L^2 + L^\infty$. For $\varphi \in C_0^\infty(\mathbb{R}^3)$, define

$$H\varphi = -\Delta\varphi + -2i\mathbf{A} \cdot \nabla\varphi - i(\nabla \cdot \mathbf{A})\varphi + V\varphi + A^2\varphi$$

Then H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$.

Proof Integration by parts shows that H is symmetric on $C_0^\infty(\mathbb{R}^3)$ and the hypotheses on V, A^2, and $\nabla \cdot \mathbf{A}$ were chosen so that, by Theorem X.15, we have $V << -\Delta$ and $\nabla \cdot \mathbf{A} << -\Delta$. We will show that $\mathbf{A} \cdot \nabla << -\Delta$,

which implies by Theorem X.12 that H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Let $\varphi \in C_0^\infty(\mathbb{R}^3)$. Suppose that $A \in L^4(\mathbb{R}^3)$. By the Hölder and Hausdorff-Young inequalities, we have

$$\begin{aligned}\left\| A^{(i)} \frac{\partial}{\partial x_i} \varphi \right\| &\leq \|A^{(i)}\|_4 \left\| \frac{\partial}{\partial x_i} \varphi \right\|_4 \\ &\leq \|A^{(i)}\|_4 \|p_i \hat{\varphi}(p)\|_{4/3} \\ &\leq \|A^{(i)}\|_4 \|(1 + |p|)^{-\alpha}\|_4 \|(1 + |p|)^{\alpha} p_i \hat{\varphi}(p)\|_2\end{aligned}$$

where we have chosen α to be any fixed number in $(\frac{3}{4}, 1)$. For any $a > 0$, there is a b so that

$$\begin{aligned}\|(1 + |p|)^{\alpha} p_i \hat{\varphi}(p)\|_2 &\leq \|(b + a|p|^2)\hat{\varphi}(p)\|_2 \\ &\leq a\|\Delta\varphi\|_2 + b\|\varphi\|_2\end{aligned}$$

by the Plancherel theorem. Thus $A^{(i)} \partial/\partial x_i << -\Delta$. A separate proof works for the L^∞ part of A. ∎

Perturbation theorems are simple and elegant and are applicable in so many cases that the test of the usefulness of any other self-adjointness method is its applicability to situations that cannot be directly handled by Theorems X.12, X.14, or X.17. One of the simplest physically interesting examples of such a situation is the **anharmonic oscillator Hamiltonian** $-d/dx^2 + x^2 + x^4$, its analogues on $\mathbb{R}^s$, and more generally the operators $-d^2/dx^2 + x^2 + x^{2m}$ $(m = 2, 3, \ldots)$. Both $H_0 = -d^2/dx^2 + x^2$ and $V = x^4$ are essentially self-adjoint on $C_0^\infty(\mathbb{R})$, but neither is a small perturbation of the other. We will use $-d^2/dx^2 + x^2 + x^4$ as a test case for many of the self-adjointness methods which we discuss later; in fact, we present five distinct proofs that $-d^2/dx^2 + x^2 + x^4$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$! All these proofs extend to prove that

$$\sum_{i=1}^{n} a_i \left(-\frac{d^2}{dx_i^2} + \omega_i^2 x_i^2 \right) + \sum_{i,j,k,\ell=1}^{n} b_{ijk\ell} x_i x_j x_k x_\ell$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ if $a_1, \ldots, a_n > 0$ and if

$$\sum_{i,j,k,\ell} b_{ijk\ell} x_i x_j x_k x_\ell \geq 0$$

for all x. All but two of them can be extended to treat the x^{2m} operators and their higher dimensional analogues. We note that the limit point–limit circle techniques discussed in the Appendix to Section X.1 can also be used to discuss the *one-dimensional* anharmonic oscillator.

There is one method of using Theorems X.12 and X.14 (the Kato–Rellich and Wüst theorems) in tandem to treat operators which are not directly amenable to perturbation theorems. The method, known as Konrady's trick, will provide our first proof that the anharmonic oscillator Hamiltonian is essentially self-adjoint on $C_0^\infty(\mathbb{R})$. Konrady's trick proves that $X + Y$ is essentially self-adjoint on some set D by a three-step process which is schematically of the following form:

(a) One finds some Z so that $X + Z$ is essentially self-adjoint on $D \subset D(X) \cap D(Z)$. Z is not a small perturbation of X. A typical example is to take Z to be a power of X and $D = C^\infty(X)$.

(b) One proves $X + Z + Y$ is essentially self-adjoint on D. Typically, this is done by proving Y is $(X + Z)$-bounded with bound less than one, so that the Kato–Rellich theorem is applicable. Notice that since Z is not a small perturbation of X, Y can be $(X + Z)$-bounded even if it is not X-bounded.

(c) One proves an estimate $\|Z\psi\| \leq \|(X + Y + Z)\psi\| + b\|\psi\|$ for some b and all $\psi \in D$. By Wüst's theorem, $X + Y = X + Y + Z - Z$ is essentially self-adjoint on D. Typically one proves this estimate (which is of the form (X.21a)) by proving the stronger estimate on operators (of the form of (X.21c)): $Z^2 \leq (X + Y + Z)^2 + b^2$.

Of course, to apply Konrady's trick, one must choose Z cleverly.

Example 6 (essential self-adjointness of $-d^2/dx^2 + x^2 + x^4$ on $C_0^\infty(\mathbb{R})$; first proof) Let $X = -d^2/dx^2 + x^2$ and $Y = x^4$. Let $Z = cX^2$ where c is a positive constant which we will choose later in the proof. Let $D = C^\infty(X) = \mathscr{S}(\mathbb{R})$. We will prove essential self-adjointness of $X + Y$ on D; the simple argument that allows one to conclude essential self-adjointness on $C_0^\infty(\mathbb{R})$ from this is left to the reader. We know that the Hermite functions (see the Appendix to Section V.3) are a complete orthonormal set for $L^2(-\infty, \infty)$ (Chapter IX, Problems 6 and 7), and that $X\psi_n = (2n + 1)\psi_n$. It follows from the Appendix to Section V.3, that $\mathrm{Ran}(X + 1) = \mathscr{S}(\mathbb{R})$, so we conclude that X is essentially self-adjoint on $\mathscr{S}$. By the spectral theorem, $X + Z$ is essentially self-adjoint on $D = C^\infty(X)$. This completes step (a) in Konrady's trick. In terms of the operators A, $A^\dagger$ introduced in Section V.3, $X = 2A^\dagger A + 1$, and $Y = \frac{1}{4}(A + A^\dagger)^4$. Using the inequality

$$\|A_1^\# \cdots A_n^\# \psi\| \leq c_n \|X^{n/2}\psi\| \tag{X.28}$$

(where each $A_j^\#$ is an A or an $A^\dagger$), one proves that $\|Y\psi\| \leq d\|X^2\psi\| \leq dc^{-1}\|(X + Z)\psi\|$. We thus pick $c = 2d$ and conclude that $X + Y + Z$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$ by employing the Kato–Rellich theorem.

This completes step (b) of Konrady's trick. Finally, let us prove that for some constant e,

$$Z^2 \leq (X + Y + Z)^2 + e \tag{X.29}$$

We compute

$$\begin{aligned}(X + Y + Z)^2 &= (X + Y)^2 + Z^2 + Z(X + Y) + (X + Y)Z \\ &= (X + Y)^2 + Z^2 + 2cX^3 + 2cXYX + 2c[X, [X, Y]] \\ &\geq Z^2 + 2cX^3 + 2c[X, [X, Y]]\end{aligned}$$

where we have used $Y \geq 0$, and $[X, [X, Y]] = X^2Y + YX^2 - 2XYX$ together with the fact that all the manipulations we perform are legitimate when applied to vectors in $\mathscr{S}(\mathbb{R})$. Finally we note that $[X, [X, Y]]$ can be written as the sum of 16 monomials of the form $A_1^{\#}A_2^{\#}A_3^{\#}A_4^{\#}$. Thus, using Theorem X.18, (X.28), and the fact that $[X, [X, Y]]$ is symmetric, we conclude

$$-[X, [X, Y]] \leq fX^2 \leq X^3 + (f + 1)$$

This proves (X.29), and thereby, applying Wüst's theorem, we conclude that $X + Y = X + Y + Z - Z$ is essentially self-adjoint on D.

We will use Konrady's trick again in Example 3 of Section X.9. (See also Problem 22.)

X.3 Positivity and self-adjointness I: Quadratic forms

We have already proven several results about positive or semibounded operators; see, for example, Theorems X.12 and X.17. In this section and the next, we exploit two different notions of positivity to prove a variety of self-adjointness theorems. In this section we use the concept of positive operator and quadratic form techniques. In the next, we use the fact that if a Hilbert space is of the form $L^2(M, d\mu)$, which is usual in applications, then it contains the distinguished cone of functions that are nonnegative a.e. Further applications of positivity conditions appear throughout this chapter, for example in Theorem X.55, and in later chapters, for example, in Section XIII.11.

It follows from the first corollary to Theorem X.1 that a semibounded symmetric operator A has equal deficiency indices, and therefore by von

Neumann's theorem, such an operator always has self-adjoint extensions. There is a distinguished extension, called the **Friedrichs extension**, which is obtained from the quadratic form associated to A.

Theorem X.23 (the Friedrichs extension) Let A be a positive symmetric operator and let $q(\varphi, \psi) = (\varphi, A\psi)$ for $\varphi, \psi \in D(A)$. Then q is a closable quadratic form and its closure $\hat{q}$ is the quadratic form of a unique self-adjoint operator $\hat{A}$. $\hat{A}$ is a positive extension of A, and the lower bound of its spectrum is the lower bound of q. Further, $\hat{A}$ is the only self-adjoint extension of A whose domain is contained in the form domain of $\hat{q}$.

Proof Let $(\varphi, \psi)_{+1} = q(\varphi, \psi) + (\varphi, \psi)$. Then $(\cdot, \cdot)_{+1}$ is an inner product on $D(A)$, so we can complete $D(A)$ under $(\cdot, \cdot)_{+1}$ to obtain a Hilbert space $\mathscr{H}_{+1}$. q clearly extends to a closed form $\hat{q}$ on $\mathscr{H}_{+1}$, but to show that $\hat{q}$ is a closed form on $\mathscr{H}$, we must show that $\mathscr{H}_{+1}$ is a subset of $\mathscr{H}$. Let i: $D(A) \to \mathscr{H}$ be the identity map. Since $\|\varphi\| \leq \|\varphi\|_{+1}$, i is bounded and thus extends by the B.L.T. theorem to a bounded map $\hat{i}$: $\mathscr{H}_{+1} \to \mathscr{H}$ of norm less than or equal to one. To show that $\mathscr{H}_{+1} \subset \mathscr{H}$, we proceed to show that $\hat{i}$ is injective. Suppose that $\hat{i}(\varphi) = 0$. Then, there exist $\varphi_n \in D(A)$ so that $\|\varphi - \varphi_n\|_{+1} \to 0$ and so that $\|\hat{i}(\varphi_n)\| = \|\varphi_n\| \to 0$. Thus

$$\begin{aligned}\|\varphi\|_{+1} &= \lim_{n, m \to \infty} (\varphi_n, \varphi_m)_{+1} \\ &= \lim_{n \to \infty} \lim_{m \to \infty} \{(\varphi_m, A\varphi_n) + (\varphi_m, \varphi_n)\} \\ &= 0\end{aligned}$$

since $\varphi_n \in D(A)$ and $\|\varphi_m\| \to 0$. Thus $\hat{i}$ is injective. Notice that the proof that $\hat{i}$ is well-defined uses only the positivity of q, but the proof that $\hat{i}$ is one to one uses the hypothesis that q arises from an operator.

Since $\hat{q}$ is closed and symmetric, by Theorem VIII.15 there is a unique self-adjoint operator $\hat{A}$ so that $D(\hat{A}) \subset Q(\hat{q})$ and $\hat{q}(\varphi, \psi) = (\varphi, \hat{A}\psi)$ if $\varphi \in Q(\hat{q})$ and $\psi \in D(\hat{A})$. Now, suppose also that $\varphi \in D(A)$. Then by the continuity of $\hat{q}$,

$$(A\varphi, \psi) = \hat{q}(\varphi, \psi) = (\varphi, \hat{A}\psi)$$

Since, this holds for all $\psi \in D(\hat{A})$, we conclude that $\varphi \in D(\hat{A}^*) = D(\hat{A})$ and $\hat{A}^*\varphi = \hat{A}\varphi = A\varphi$. Thus $\hat{A}$ extends A. The same proof shows that if A_e is any symmetric extension of A with $D(A_e) \subset Q(\hat{q})$, then $\hat{A}$ extends A_e. Thus if A_e is self-adjoint $\hat{A} = A_e$.

The easy proof of the statement about the spectrum of A is left to the reader. ∎

In Section VIII.6 we proved that the quadratic form $q(\varphi, \psi) = \overline{\varphi(0)}\psi(0)$ on $C_0^\infty(\mathbb{R})$ is not closable. In the terminology of the above proof, the reason is that $\mathscr{H}_{+1} = \{\langle \psi, a\rangle | \psi \in L^2(\mathbb{R}), a \in \mathbb{R}\}$ where a is the "value" of ψ at zero. Thus the map i: $\langle \psi, a\rangle \to \psi$ is not 1–1.

Two nice features of the Friedrichs extensions are the preservation of the lower bound and the fact that the domain of $\hat{A}$ is contained in the form domain of $\hat{q}$. In certain cases one can say more about the domain of $\hat{A}$; see the Notes and Theorem X.32.

Example 1 Let $A = -d^2/dx^2$ on $C_0^\infty(0, 1)$. Then

$$\|\psi\|_{+1}^2 = \|d\psi/dx\|^2 + \|\psi\|^2$$

If $\psi_n \xrightarrow{\|\cdot\|_{+1}} \psi$, then ψ has an L^2 derivative. It easily follows that

$$|\psi_n(a) - \psi(a)| \to 0$$

for each $a \in [0, 1]$. Thus for all $\varphi \in D(\hat{A})$, $\varphi(0) = 0 = \varphi(1)$, i.e., the Friedrichs extension $\hat{A}$ of $-d^2/dx^2$ is the self-adjoint extension with boundary conditions $\varphi(0) = 0 = \varphi(1)$. The spectrum of this extension is $\{(n\pi)^2 | n = 1, 2, \ldots\}$ with corresponding eigenfunctions $\{\sin(n\pi x)\}$. Since $\hat{A}$ is bounded below by π, the same must be true of the original quadratic form arising from A. Thus, by an integration by parts we conclude the classical inequality

$$\int_0^1 |\varphi'(x)|^2 \, dx \geq \pi^2 \int_0^1 |\varphi(x)|^2 \, dx$$

for functions $\varphi \in C_0^\infty(0, 1)$. We remark that this can also be computed directly by using Fourier series. Notice that another self-adjoint extension of A may have a smaller lower bound than $\hat{A}$. For example, the self-adjoint extension with boundary conditions $\varphi'(0) = 0 = \varphi'(1)$ has lower bound zero. On the other hand, it is possible for a self-adjoint extension other than the Friedrichs extension to have the same lower bound as the Friedrichs extension. For example, the self-adjoint extension $\tilde{A}$ with boundary conditions $\varphi(0) = -\varphi(1)$, $\varphi'(0) = -\varphi'(1)$ has eigenvalues $(n\pi)^2$, $n = 1, 3, \ldots$, each of multiplicity 2.

Let A_0 be the extension of A with boundary conditions $\varphi(0) = 0 = \varphi(1)$, $\varphi'(0) = -\varphi'(1)$. The reader can easily check that A_0 has deficiency indices $\langle 1, 1\rangle$. Clearly, both $\hat{A}$ and $\tilde{A}$ extend A_0. So, even in the case of deficiency indices $\langle 1, 1\rangle$, another self-adjoint extension may have the same lower bound as the Friedrichs extension.

Example 2 (weak solutions of partial differential equations) Let Ω be an open region in $\mathbb{R}^n$ and let A be the operator $-\Delta + I$ with domain $C_0^\infty(\Omega) \subset L^2(\Omega)$. A is symmetric and bounded below by one. If $\hat{A}$ is the Friedrichs extension of A, then $\hat{A} \geq I$ also, so $\mathrm{Ran}(\hat{A}) = L^2(\Omega)$. Thus, for any $g \in L^2(\Omega)$, there is an $f \in D(\hat{A})$ so that $\hat{A}g = f$. So, if $\varphi \in C_0^\infty(\Omega)$,

$$(\varphi, g) = (\varphi, \hat{A}f) = (\hat{A}\varphi, f) = ((-\Delta + I)\varphi, f)$$

That is, for each $g \in L^2(\Omega)$, the equation

$$(-\Delta + I)f = g$$

has a weak solution $f \in L^2(\Omega)$. Since $\Delta f = f - g \in L^2(\Omega)$, we can use Sobolev's lemma (Section IX.6) to show a certain amount (depending on n) of regularity for f. If $g \in C_0^\infty(\Omega)$, then applying Δ repeatedly to the equation $\Delta f = f - g$ proves that $f \in \bigcap_{m=1}^\infty W_m(\Omega)$, so in this case Sobolev's lemma implies that f is a C^∞ function.

For another application of the Friedrichs extension, see Problem 25 where the reader is asked to prove the Stieltjes moment condition, the analogue of the Hamburger condition when $[0, \infty)$ replaces $(-\infty, \infty)$. In this application, as in the above example, it is crucial that the Friedrichs extension of A has the same lower bound as A. This suggests the problem of investigating the lower bounds of the other self-adjoint extensions.

Proposition Let A be a semibounded symmetric operator with finite deficiency indices. Then any self-adjoint extension of A is bounded below (possibly with a smaller lower bound).

Proof Let $\tilde{A}$ be a self-adjoint extension of A with corresponding projection-valued measure P_Ω. Suppose that the deficiency indices of A equal n. Then by Theorem X.2, $D(\tilde{A}) = D(A) + S$ where S is an n-dimensional vector space. Let K be less than M, the lower bound of A. Then we must have $\dim P_{(K,M)} \leq n$. Otherwise we could find a vector in $D(A) \cap \mathrm{Ran}\, P_{(K,M)}$, which would contradict the fact that A is bounded below by M. Thus, $\dim P_{(-\infty,M)} \leq n$, so $\tilde{A}$ is bounded below. ∎

In the case of infinite deficiency indices, a semibounded symmetric operator can have self-adjoint extensions that are not bounded below (Problem 26). But even in this case there will always be many self-adjoint extensions that are bounded below. In fact, unless A is already essentially self-adjoint, there will be other extensions besides the Friedrichs extension which are bounded from below.

Theorem X.24 Let A be a symmetric operator that is bounded from below. If the Friedrichs extension $\hat{A}$ is the only self-adjoint extension of A that is bounded from below, then A is essentially self-adjoint.

Proof By the proposition, we need only consider the case where the deficiency indices of A equal infinity. Suppose $\hat{A}$ is the Friedrichs extension of A and let $\tilde{A}$ be a symmetric extension of A contained in $\hat{A}$ which has deficiency indices equal to one (to see how to construct such an A, consult Theorem X.2). Then A is bounded from below, so by the proposition all its self-adjoint extensions will be bounded from below. Hence A has more than one semibounded self-adjoint extension unless its deficiency indices are equal to zero. ∎

Another application of positivity and quadratic form techniques is the following theorem of von Neumann. His original operator-theoretic proof does not use quadratic forms.

Theorem X.25 Let A be a *closed* densely defined operator and let

$$D(A^*A) = \{\psi \in D(A) \,|\, A\psi \in D(A^*)\}$$

Define A^*A on $D(A^*A)$ by $(A^*A)\psi = A^*(A\psi)$. Then A^*A is self-adjoint.

Proof Define the form $b(\varphi, \psi)$ on $D(A) \times D(A)$ by $b(\varphi, \psi) = (A\varphi, A\psi)$. b is nonnegative and since A is closed as an operator, b is closed as a quadratic form. Let B be the associated self-adjoint operator given by Theorem VIII.15. We will show that $B = A^*A$. Notice that, a priori, it is not evident that there are any vectors besides the zero vector in $D(A^*A)$.

Let $\mathscr{H}_{+1} \subset \mathscr{H} \subset \mathscr{H}_{-1}$ be the scale of spaces defined by b as in the proof of Theorem VIII.15. Define $\hat{A}^*: \mathscr{H} \to \mathscr{H}_{-1}$ by $(\hat{A}^*\varphi)(\psi) = (\varphi, A\psi)$. By the definition of adjoint $D(A^*) = \{\varphi \,|\, \hat{A}^*\varphi \in \mathscr{H}\}$ and $A^* = \hat{A}^* \restriction D(A^*)$. Let $\hat{B}: \mathscr{H}_{+1} \to \mathscr{H}_{-1}$ be the natural map given by $(\hat{B}\varphi, \psi) = b(\varphi, \psi)$. From the proof of Theorem VIII.15, we have that $D(B) = \{\varphi \in \mathscr{H}_{+1} \,|\, \hat{B}\varphi \in \mathscr{H}\}$ and $B = \hat{B} \restriction D(B)$. Now, suppose $\varphi, \psi \in \mathscr{H}_{+1}$. Then

$$[\hat{A}^*(A\varphi)](\psi) = (A\varphi, A\psi) = (\hat{B}\varphi)(\psi)$$

so $\hat{B} = \hat{A}^*A$. Thus

$$\begin{aligned} D(B) &= \{\varphi \in \mathscr{H}_{+1} \,|\, \hat{B}\varphi \in \mathscr{H}\} \\ &= \{\varphi \in \mathscr{H}_{+1} \,|\, A^*(A\varphi) \in \mathscr{H}\} \\ &= \{\varphi \in \mathscr{H}_{+1} \,|\, A\varphi \in D(A^*)\} \\ &= D(A^*A) \end{aligned}$$

and $B = \hat{B} \restriction D(B) = A^*A$. ∎

The proof has the following corollary.

Corollary Let A be a closed operator. Then any core for A is a form core for A^*A.

Corollary If A is symmetric and A^2 is densely defined, then A^*A is the Friedrichs extension of A^2.

Example 3 Let $A = i\,d/dx$ with domain

$$D(A) = \{\varphi \,|\, \varphi \in AC[0, 1], \varphi(0) = \varphi(1) = 0\}$$

We have already computed that

$$D(A^*) = \{\varphi \,|\, \varphi \in AC[0, 1]\}$$

and $A^*\varphi = i\,d\varphi/dx$. It follows immediately from the definitions of $D(AA^*)$ and $D(A^*A)$ and the above theorem that A^*A is the self-adjoint extension of $-d^2/dx^2$ with boundary conditions $\varphi(0) = 0 = \varphi(1)$, and AA^* is the self-adjoint extension of $-d^2/dx^2$ with boundary conditions $\varphi'(0) = 0 = \varphi'(1)$.

Example 4 (Schrödinger operators with magnetic fields) One can use quadratic form methods to define self-adjoint Hamiltonians of the form of (X.26) although not with explicit control over operator domains. Consider first the case $V = 0$. Suppose that $\mathbf{A} \in L^2(\mathbb{R}^3)_{\text{loc}}$. Let T_j denote the closure of the symmetric operator $-i^{-1}\,\partial/\partial x_j + eA_j/c$ on $C_0^\infty(\mathbb{R}^3)$. A simple extension of Theorem X.25 shows that $H = \sum_{i=1}^3 T_i^* T_i$ can be defined as a self-adjoint operator on

$$\left\{\psi \in \bigcap_{i=1}^3 D(T_i) \,\middle|\, T_i\psi \in D(T_i^*)\right\}$$

The same method works if $V \geq 0$ with $V \in L^1_{\text{loc}}$. In either case one has

$$Q(H) = \left(\bigcap_{i=1}^3 D(T_i)\right) \cap Q(V)$$

In the next section we will describe $D(-\Delta + V)$ when $V \geq 0$ and $V \in L^1_{\text{loc}}$.

We conclude this section by summarizing in one place some of the facts which we have proven about strictly positive symmetric operators. Of course every semibounded symmetric operator becomes strictly positive after translation by a constant.

Theorem X.26 Let A be a strictly positive symmetric operator, i.e. $(A\varphi, \varphi) \geq c(\varphi, \varphi)$ for all $\varphi \in D(A)$ and some $c > 0$. Then the following are equivalent:

(a) A is essentially self-adjoint.
(b) $\mathrm{Ran}(A)$ is dense.
(c) $\mathrm{Ker}(A^*) = \{0\}$.
(d) A has only one semibounded self-adjoint extension.

X.4 Positivity and self-adjointness II: Pointwise positivity

The results of the previous section depended on exploiting the notion of positive operator, something which makes sense on any Hilbert space $\mathscr{H}$. In this section, we exploit a different type of positivity associated with L^2 spaces—that of a vector being positive. This is not a notion intrinsic to $\mathscr{H}$ alone but to its realization as an L^2 space. This notion will appear again from time to time and will play a major role in Section XIII.11. Since the Hilbert space of quantum mechanics is typically given as an L^2 space, there is present in such cases the structure associated with positive vectors. Given the positive vectors, there is an associated notion of positive multiplication operator, i.e., a multiplication operator $\psi(x) \mapsto V(x)\psi(x)$ which takes the positive vectors into themselves. The major results in this section concern the essential self-adjointness of $-\Delta + V$ if $V \geq 0$ under very weak additional assumptions, and of magnetic field Schrödinger Hamiltonians in a general situation.

First, we extend the notion of positivity to distributions:

Definition Let $T \in \mathscr{D}'(\mathbb{R}^n)$. We say that T is **positive** and write $T \geq 0$ if and only if $T(f) \geq 0$ whenever $f \in \mathscr{D}$ is pointwise nonnegative. If $T, S \in \mathscr{D}$ and $T - S \geq 0$, we write $T \geq S$.

We immediately note two facts about positive distributions. First, if $T(f) = \int F(x) f(x)\, d^n x$ where F is a continuous function on $\mathbb{R}^n$, then $T \geq 0$ if and only if $F(x) \geq 0$ for all x. Secondly, if T_n is a sequence of positive distributions and $T_n \to T$ weakly, then T is positive.

Our self-adjointness result depends on the following elegant distributional inequality:

Theorem X.27 (Kato's inequality) Let u be a locally L^1 function on $\mathbb{R}^n$ whose distributional Laplacian Δu is also a locally L^1 function. Define

$$(\operatorname{sgn} u)(x) = \begin{cases} 0 & \text{if } u(x) = 0 \\ \overline{u(x)}/|u(x)| & \text{if } u(x) \neq 0 \end{cases}$$

so that $\operatorname{sgn} u$ is L^∞ and $(\operatorname{sgn} u)\,\Delta u$ is a locally L^1 function and hence a distribution. Then the distributional Laplacian $\Delta|u|$ of $|u|$ obeys the following distributional inequality:

$$\Delta|u| \geq \operatorname{Re}[(\operatorname{sgn} u)\,\Delta u] \tag{X.30}$$

Example 1 To help understand this result, consider the case $n = 1$ where $u \in C^\infty(\mathbb{R})$ is strictly positive if $x > 0$ and strictly negative if $x < 0$. Then $|u|$ is C^∞ on $\mathbb{R}\backslash\{0\}$, but at $x = 0$ its first derivative has a discontinuity of magnitude $2u'(0)$. Thus

$$\frac{d^2}{dx^2}|u| = (\operatorname{sgn} u)\frac{d^2}{dx^2}u + 2u'(0)\,\delta(x)$$

so we can see (X.30) explicitly since $u'(0) \geq 0$.

Proof of Theorem X.27 Suppose first that u is C^∞ and let u_ε be given by

$$u_\varepsilon(x) = \sqrt{|u(x)|^2 + \varepsilon^2} \tag{X.31}$$

so that u_ε is C^∞. Differentiating the square of (X.31),

$$2u_\varepsilon(x)[\operatorname{grad} u_\varepsilon(x)] = 2\operatorname{Re}[\overline{u(x)}(\operatorname{grad} u(x))] \tag{X.32}$$

Since (X.31) implies that $|u_\varepsilon| \geq |u|$, (X.32) implies that

$$|\operatorname{grad} u_\varepsilon| \leq |\overline{u(x)}|\,|u_\varepsilon(x)|^{-1}|\operatorname{grad} u(x)| \leq |\operatorname{grad} u(x)| \tag{X.33}$$

Taking the divergence of (X.32) we see that

$$u_\varepsilon\,\Delta u_\varepsilon + |\operatorname{grad} u_\varepsilon|^2 = \operatorname{Re}(\bar{u}\,\Delta u) + |\operatorname{grad} u|^2$$

so on account of (X.33)

$$u_\varepsilon\,\Delta u_\varepsilon \geq \operatorname{Re}(\bar{u}\,\Delta u)$$

pointwise and thus in distributional sense.

As a result,

$$\Delta u_\varepsilon \geq \operatorname{Re}(\operatorname{sgn}_\varepsilon(u)\,\Delta u) \tag{X.34}$$

where

$$\operatorname{sgn}_\varepsilon(u(x)) = \overline{u(x)}/u_\varepsilon(x)$$

Now let u be an arbitrary locally L^1 function with $\Delta u \in L^1_{\text{loc}}$ and let j_δ be an approximate identity, i.e., let $j_\delta(x) = j(x/\delta)\delta^{-n}$ where $j \geq 0$, $j \in C_0^\infty(\mathbb{R}^n)$ and $\int j(x)\, d^n x = 1$. Let $u^\delta = u * j_\delta$. Since u^δ is C^∞,

$$\Delta(u^\delta)_\varepsilon \geq \text{Re}(\text{sgn}_\varepsilon(u^\delta)\, \Delta u^\delta) \tag{X.35}$$

for each ε, $\delta > 0$. Fix $\varepsilon > 0$ and take $\delta \to 0$. Then $u^\delta \to u$ in local L^1 norm and thus also in $\mathscr{D}'$. In particular, by passing to a subsequence, we can suppose that $u^\delta(x) \to u(x)$ pointwise a.e. Thus $\text{sgn}_\varepsilon(u^\delta) \to \text{sgn}_\varepsilon(u)$ pointwise a.e. Since $\Delta u^\delta = (\Delta u)^\delta$ and Δu is also in L^1_{loc}, $\Delta u^\delta \to \Delta u$ in L^1_{loc}. It is now easy to see that $\text{sgn}_\varepsilon(u^\delta)\, \Delta u^\delta \to \text{sgn}_\varepsilon(u)\, \Delta u$ in $\mathscr{D}'$, so taking $\delta \to 0$ in (X.35) we conclude that (X.34) holds for u. Now take $\varepsilon \to 0$. Then $\text{sgn}_\varepsilon(u) \to \text{sgn}(u)$ pointwise with a uniform bound ($|\text{sgn}_\varepsilon u| \leq 1$), so that the two sides of (X.34) converge in $\mathscr{D}'$ to the two sides of (X.30). ∎

Typical of the applications of Theorem X.27 is

Theorem X.28 Let $V \in L^2(\mathbb{R}^n)_{\text{loc}}$ with $V \geq 0$ pointwise. Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Proof By Theorem X.26, we need only show that

$$(-\Delta + V + 1)^* u = 0 \tag{X.36}$$

implies that $u = 0$. But by the fact that $-\Delta + V$ is given with domain C_0^∞, (X.36) is equivalent to

$$(-\Delta + V + 1)u = 0, \qquad u \in L^2(\mathbb{R}^n) \tag{X.37}$$

where the derivative in question is a distributional derivative. (X.35) implies that $\Delta u = Vu + u$ is in L^1_{loc} since u and $V + 1$ are in L^2_{loc}. Thus, by Theorem X.27

$$\Delta|u| \geq \text{Re}(\text{sgn}\, u\, \Delta u) = \text{Re}(\text{sgn}\, u\, (Vu + u)) = (V + 1)|u| \tag{X.38}$$

In particular, $\Delta|u| \geq 0$.

Let j_δ be an approximate identity, as in the previous theorem, and let $w = |u|$, $w^\delta = w * j^\delta$. Then $\Delta w^\delta = w * \Delta j_\delta \in L^2$, so w^δ is in $D(\Delta)$ and thus $(w^\delta, \Delta w^\delta) \leq 0$ with equality only if $w^\delta = 0$. But $\Delta w^\delta = \Delta|u| * j_\delta \geq 0$ in distributional sense and so $\Delta w_\delta \geq 0$ pointwise. Thus, $(w^\delta, \Delta w^\delta) \geq 0$ so $w^\delta = 0$. Since $w^\delta \to w$ as $\delta \to 0$, $w = 0$ and therefore $u = 0$. ∎

Example 2 (essential self-adjointness of $-d^2/dx^2 + x^2 + x^4$ on $C_0^\infty(\mathbb{R})$; second proof) Since $x^2 + x^4$ is positive, and locally L^2, Theorem X.28

implies that $-d^2/dx^2 + x^2 + x^4$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$. More generally, $-\Delta + P(x_1, \ldots, x_n)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ for any polynomial bounded from below.

Example 3 Let $V(x) = 2|x|^{-2}$ on $L^2(\mathbb{R}^5)$. Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$ by Theorem X.28 (or by Theorem X.11). On the other hand, $V \in L^2_{\text{loc}}$ and $-\Delta - V$ is bounded below but not essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$ (see Theorem X.11 and Example 4 in Section X.2). Thus the condition $V \geq 0$ in Theorem X.28 cannot be completely eliminated.

Theorem X.28 can be extended in a variety of ways.

Theorem X.29 Let $V = V_1 + V_2$ where $V_1 \geq 0$, $V_1 \in L^2(\mathbb{R}^n)_{\text{loc}}$ and where V_2 is a $-\Delta$-bounded multiplication operator with relative bound $a < 1$. Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. In particular, if V is a multiplication operator with $V_+ = \max(V, 0) \in L^2_{\text{loc}}$ and $V_- = \min(V, 0) \in L^p + L^\infty$ where $p = 2$ if $n \leq 3$, $p > 2$ if $n = 4$ and $p = n/2$ if $n \geq 5$, then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Proof By following the arguments in Theorem X.28, we need only show that $(-\Delta + V + b)u = 0$ (distributional sense) and $u \in L^2(\mathbb{R}^n)$ implies that $u = 0$, where b is some large constant to be chosen below. Since $C_0^\infty(\mathbb{R}^n) \subset D(-\Delta) \subset D(V_2)$, V_2 is in L^2_{loc}; so by using Kato's inequality, we obtain the analogue of (X.38)

$$\Delta|u| \geq (V + b)|u| \geq (V_2 + b)|u|$$

Thus

$$(-\Delta + b)|u| \leq -V_2|u| \tag{X.39}$$

Now, by the explicit form of its kernel (Problem 50 of Chapter IX), $(-\Delta + b)^{-1}$ takes positive elements of $\mathscr{S}(\mathbb{R}^n)$ into other positive elements; and so, since it is self-adjoint, positive elements of $\mathscr{S}'(\mathbb{R}^n)$ into other positive tempered distributions. Moreover, since V_2 is $-\Delta$-bounded

$$\left| \int V_2(x)|u(x)| f(x)\, dx \right| \leq (\text{const})\|u\|_{L^2}\|(-\Delta + 1)f\|$$

so $V_2|u|$ is a tempered distribution. Thus by (X.39),

$$|u| \leq -(-\Delta + b)^{-1} V_2|u| \tag{X.40}$$

Since V_2 has $-\Delta$ bound $a < 1$, we can choose b so that $\|(-\Delta + b)^{-1} V_2\| \leq \frac{1}{2}(a + 1) < 1$. Then by (X.40)

$$\|u\| \leq \|(-\Delta + b)^{-1} V_2\| \, \|u\|$$

so $\|u\| = 0$. ∎

We state without proof the following theorem which generalizes part of Theorem X.11 to the noncentral case:

Theorem X.30 (Kalf-Walter-Schmincke-Simon theorem) Let $V = V_1 + V_2$ with $V_2 \in L^\infty(\mathbb{R}^n)$ and $V_1 \in L^2(\mathbb{R}^n \backslash \{0\})_{\text{loc}}$ obeying

$$V_1(\mathbf{r}) \geq -n(n-4)/4r^2$$

Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \backslash \{0\})$.

References to the proof which exploits Kato's inequality can be found in the Notes.

There is another proof of Theorem X.29 which is of interest because it exploits the following very beautiful result about positivity in L^2 spaces:

Definition A bounded operator A on $L^2(X, d\mu)$ is called **positivity preserving** if $(A\varphi)(x) \geq 0$ a.e. whenever $\varphi(x) \geq 0$ a.e. A semigroup $T(t)$ is called positivity preserving if it is positivity preserving for each $t \geq 0$.

Theorem X.31 (the Davies-Faris theorem) Let H_0 be a positive self-adjoint operator on $L^2(X, d\mu)$ such that e^{-tH_0} is positively preserving. Let V be a multiplication operator with $V \geq 0$. Suppose that $H = H_0 + V$ is essentially self-adjoint on $D(H_0) \cap D(V)$. Let W be an H_0-bounded multiplication operator. Then W is H-bounded. In fact, if

$$\|W\psi\| \leq a\|(H_0 + b)\psi\| \qquad \text{all} \quad \psi \in D(H_0)$$

then

$$\|W\psi\| \leq a\|(H + b)\psi\| \qquad \text{all} \quad \psi \in D(H)$$

Proof Suppose that $\|W(H_0 + b)^{-1}\| \leq a$. We will show that

$$\|W(H + b)^{-1}\| \leq a$$

Since e^{-tH_0} is positivity preserving, so is $(H_0 + b)^{-1} = \int_0^\infty e^{-bt}e^{-tH_0}\,dt$. Also, by the Trotter product formula, $e^{-tH} = s - \lim_{n\to\infty}(e^{-tH_0/n}e^{-tV/n})^n$ is positivity preserving, and, so by the same argument, $(H + b)^{-1}$ is positivity preserving. We will prove later (see Theorem X.55) that if A is bounded and positivity preserving, then $|A\psi| \le A|\psi|$ pointwise for all ψ. Thus we need only prove that

$$\|W(H + b)^{-1}|\psi|\| \le a\|\psi\|$$

for all ψ. If we can show that (pointwise)

$$0 \le (H + b)^{-1}\varphi \le (H_0 + b)^{-1}\varphi \tag{X.41a}$$

for all $\varphi \ge 0$, it follows that (pointwise)

$$0 \le |W|(H + b)^{-1}\varphi \le |W|(H_0 + b)^{-1}\varphi \tag{X.41b}$$

and

$$\|W(H + b)^{-1}|\psi|\| \le a\|\psi\|$$

for all ψ.

So suppose that $\varphi \ge 0$. Then, since $|e^{-sV}| \le 1$ and e^{-sH_0} is positivity preserving,

$$e^{-sH_0}(1 - e^{-sV})\varphi \ge 0$$

so

$$0 \le (e^{-sH_0}e^{-sV})\varphi \le e^{-sH_0}\varphi \tag{X.42}$$

Iterating (X.42), we get

$$0 \le (e^{-t/nH_0}e^{-t/nV})^n\varphi \le e^{-tH_0}\varphi$$

So by the Trotter product formula

$$0 \le e^{-tH}\varphi \le e^{-tH_0}\varphi \tag{X.43}$$

(X.41b) follows from (X.43) by the Laplace transform formula for $(H + b)^{-1}$ in terms of e^{-tH}. ∎

As a corollary of the Davies–Faris theorem we have:

Second Proof of Theorem X.29 By Theorem X.28, $-\Delta + V_1$ is essentially self-adjoint on $D(\Delta) \cap D(V_1)$. Moreover, $e^{t\Delta}$ is positivity preserving on account of its explicit kernel (IX.31). Thus, by hypothesis, and Theorem X.31, V_2 is $-\Delta + V_1$ bounded with bound less than 1, so $-\Delta + V_1 + V_2$ is essentially self-adjoint on any core for $-\Delta + V_1$ by the Kato–Rellich theorem. ∎

Kato's inequality can also be used to study $D(-\Delta + V)$ when $-\Delta + V$ is defined as a sum of quadratic forms:

Theorem X.32 Let $V \geq 0$ be in $L^1_{\text{loc}}(\mathbb{R}^n)$. Let $H = -\Delta + V$ defined as a sum of quadratic forms. Then $D(H)$ equals

$$\{\varphi \in L^2(\mathbb{R}^n) \,|\, V\varphi \in L^1_{\text{loc}} ; (-\Delta\varphi + V\varphi)_{\text{dist}} \in L^2\} \tag{X.44}$$

where $(-\Delta\varphi + V\varphi)_{\text{dist}}$ means the distribution $f \to \int \varphi(-\Delta f) + \int (V\varphi) f$. Moreover, $H\varphi = (-\Delta\varphi + V\varphi)_{\text{dist}}$.

Proof Let T be the operator with domain (X.44) and $T\varphi = -\Delta\varphi + V\varphi$. We first claim that T extends H. For let $\varphi \in D(H) \subset Q(H) = Q(-\Delta) \cap Q(V)$. Since $\varphi \in Q(V)$ we have $|V|^{1/2}\varphi \in L^2$ and since $|V|^{1/2} \in L^2_{\text{loc}}$, we conclude that $V\varphi \in L^1_{\text{loc}}$. Moreover $H\colon \mathscr{H}_{+1} \to \mathscr{H}_{-1}$ is $-\Delta + V$ defined in the distributional sense, so by the construction of $D(H)$ in Theorem VIII.15, $H\varphi = -\Delta\varphi + V\varphi \in L^2$, i.e., $\varphi \in D(T)$ and $H\varphi = T\varphi$.

Suppose now that $\eta \in D(T)$. Since H is self-adjoint and positive, we can find $\varphi \in D(H)$ with $(T + 1)\eta = (H + 1)\varphi$. Let $\psi = \eta - \varphi$. Then, since T extends H, $(T + 1)\psi = 0$. Since $\psi \in D(T)$ we have that $-\Delta\psi = T\psi - V\psi = -\psi - V\psi \in L^1_{\text{loc}}$, so Kato's inequality is applicable and assures us that

$$\Delta|\psi| \geq (\operatorname{sgn}\psi)(\psi + V\psi) = (V + 1)|\psi| \geq 0$$

As in the proof of Theorem X.28, this implies that $\psi = 0$. Thus $\eta = \varphi \in D(H)$, i.e., $D(T) \subset D(H)$. So $T = H$. ∎

Next, we turn to the application of Kato's inequality to Schrödinger operators with magnetic fields. We first need a more general version of the inequality:

Theorem X.33 Let a_k $(k = 1, \ldots, n)$ be real-valued functions in $C^1(\mathbb{R}^n)$. Let D_k be the operator on $\mathscr{D}'$

$$D_k T = \frac{1}{i}\frac{\partial T}{\partial x_k} - a_k T$$

and let $D^2 = \sum D_k^2$. Then, for any u with $u \in L^1_{\text{loc}}$ and $D^2 u \in L^2_{\text{loc}}$,

$$\Delta|u| \geq -\operatorname{Re}[(\operatorname{sgn} u) D^2 u] \tag{X.45}$$

The main additional idea needed to prove Theorem X.33, given the proof of Theorem X.27, is:

Lemma Under the hypotheses of Theorem X.33, Δu and ∇u are in L^1_{loc}.

Proof We need only show that Δu, ∇u are locally L^1 near $x = 0$. Let f be a function in C_0^∞, identically 1 near 0. Then by explicit computation

$$(-\Delta + 1)(fu) = h_1 + \nabla \cdot \mathbf{h}_2 \tag{X.46}$$

with

$$h_1 = fD^2u + (\Delta f)u + if(\nabla \cdot \mathbf{a})u - 2i(\nabla f) \cdot \mathbf{a}u + (a^2 + 1)fu$$
$$\mathbf{h}_2 = 2if\mathbf{a}u - 2(\nabla f)u$$

What is important is that by hypothesis, $h_1 \in L^1$, $\mathbf{h}_2 \in L^2$, and $fu \in L^2$. Thus, all the functions in (X.46) lie in $\mathscr{S}'(\mathbb{R}^n)$. Since $(-\Delta + 1)$ is invertible on $\mathscr{S}$, it is invertible on $\mathscr{S}'$, so that

$$fu = (-\Delta + 1)^{-1}h_1 + (-\Delta + 1)^{-1}\nabla \cdot \mathbf{h}_2$$

and

$$\nabla(fu) = \nabla(-\Delta + 1)^{-1}h_1 + \nabla(-\Delta + 1)^{-1}\nabla \cdot \mathbf{h}_2$$

Now, since $\mathbf{h}_2 \in L^2$, its Fourier transform is in L^2 so that

$$\nabla_i(-\Delta + 1)^{-1}\nabla \cdot \mathbf{h}_2 = \mathscr{F}^{-1}\left(p_i(p^2 + 1)^{-1}\sum_j p_j \cdot \hat{h}_j\right)$$

is in L^2 since $p_i p_j(p^2 + 1)^{-1} \in L^\infty$. Let $G_i(x)$ be the distribution with $\hat{G}_i(p) = (2\pi)^{-n/2}p_i(p^2 + 1)^{-1}$. By following the methods of Problem 50 of Chapter IX, $G_i(x)$ is continuous away from $x = 0$, falling exponentially at infinity and $|G_i(x)| \leq C|x|^{-n+1}$ ($\ln|x|$ if $n = 1$). Thus $G_i \in L^p$ for some $p > 1$ and therefore $G_i * h_1 \in L^p$ by Young's inequality. We conclude that $\nabla(fu)$ lies in L^1_{loc} and so ∇u is L^1_{loc} near 0. Now, since $\nabla u \in L^1_{\text{loc}}$, we conclude that $\nabla \cdot \mathbf{h}_2 \in L^1_{\text{loc}}$ so by (X.46), $-\Delta u \in L^1_{\text{loc}}$. ∎

Proof of Theorem X.33 Suppose first that $u \in C^\infty(\mathbb{R}^n)$ and let u_ε be given by (X.31). Then since $\text{Im}\overline{(u(x)}a_j(x)u(x)) = 0$, (X.32) implies that

$$u_\varepsilon \operatorname{grad}_k u_\varepsilon = \text{Re}[\overline{u(x)}(iD_k u)(x)] \tag{X.47}$$

so that

$$|\operatorname{grad} u_\varepsilon| \leq |Du| \tag{X.48}$$

Taking the divergence of (X.47) and using

$$\begin{aligned}\partial_k[\bar{u}(iD_k u)] &= (\partial_k \bar{u})(iD_k u) + \bar{u}(\partial_k(iD_k u)) \\ &= \overline{[(\partial_k - ia_k)u]}(iD_k u) + \bar{u}(\partial_k - ia_k)(iD_k u) \\ &= |D_k u|^2 - \bar{u}D_k^2 u\end{aligned}$$

we see that

$$\Delta u_\varepsilon \geq -\mathrm{Re}[\mathrm{sgn}_\varepsilon(u) D^2 u] \tag{X.49}$$

We have used (X.48) as in the proof of Theorem X.27. As in that proof, we now approximate a given $u \in L^2_{\mathrm{loc}}$ with $D^2 u \in L^1_{\mathrm{loc}}$ by u^δ's. Since, by the lemma, $u \in L^2_{\mathrm{loc}}$ and $D^2 u \in L^1_{\mathrm{loc}}$ imply that Δu and $\nabla u \in L^1_{\mathrm{loc}}$, we conclude that $D^2 u^\delta \to D^2 u$ in L^1_{loc}. Thus (X.49) holds for any u obeying the hypothesis of the theorem. (X.45) follows from (X.49) by letting ε approach 0. ∎

Theorem X.34 Let $a_k \in C^1(\mathbb{R}^n)$. Let $V = V_1 + V_2$ with V_1, V_2 obeying the hypotheses of Theorem X.29. Then

$$H = -\sum_{j=1}^{n} \frac{1}{2m_j} (\partial_j - i a_j)^2 + V$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Proof One just follows the proof of Theorem X.29 using (X.45) in place of (X.30), noting that the u to which we want to apply (X.45) is in L^2_{loc} and not merely in L^1_{loc}. ∎

Example 4 (the Zeeman effect) Let $\mathbf{a}(\mathbf{x}) = \frac{1}{2}\mathbf{x} \times \mathbf{B}_0$ where $\mathbf{B}_0$ is constant. The Hamiltonian of an N-electron atom in a constant external magnetic field is

$$H = -\frac{1}{2M}(\partial_0 - iNe\mathbf{a}(\mathbf{x}_0)/c)^2 - \frac{1}{2m}\sum_{n=1}^{N}(\partial_n + ie\mathbf{a}(\mathbf{x}_n)/c)^2$$
$$-\sum_{n=1}^{N}\frac{Ne^2}{|\mathbf{x}_n - \mathbf{x}_0|} + \frac{1}{2}\sum_{n\neq m}\frac{e^2}{|\mathbf{x}_n - \mathbf{x}_m|}$$

By Theorem X.34, H is essentially self-adjoint of $C_0^\infty(\mathbb{R}^{3N+3})$.

One can considerably weaken the smoothness hypotheses on $\mathbf{a}$ if one imposes the **Coulomb gauge condition**, $\mathrm{div}\,\mathbf{a} = 0$ (distributional sense). Notice in that case

$$D^2 u = -\Delta u - 2i\mathbf{a}\cdot\nabla u + \mathbf{a}^2 u$$

so that one can define D^2 on C_0^∞ without any smoothness hypothesis on $\mathbf{a}$; only $a \in L^4_{\mathrm{loc}}$ is needed. The extra condition $\mathrm{div}\,\mathbf{a} = 0$ is quite common in the physics literature. To explain why, let us proceed formally. Given

$\lambda(x)$, let $\tilde{\mathbf{a}} = \mathbf{a} + \operatorname{grad} \lambda$. Notice that this does not change the magnetic field $\mathbf{B} = \operatorname{curl} \mathbf{a}$, i.e., $\operatorname{curl} \mathbf{a} = \operatorname{curl} \tilde{\mathbf{a}}$. If $\tilde{\mathbf{D}} = (i\partial - \tilde{\mathbf{a}})$, then

$$\tilde{\mathbf{D}} = e^{-i\lambda} \mathbf{D} e^{+i\lambda}$$

so that

$$e^{-i\lambda}(-D^2 + V)e^{+i\lambda} = -\tilde{D}^2 + V$$

Thus $-D^2 + V$ and $-\tilde{D}^2 + V$ are formally unitarily equivalent and the gauge transformation $\mathbf{a} \mapsto \tilde{\mathbf{a}}$ does not change the magnetic field. If λ is not C^∞, $-\tilde{D}^2 + V$ may have $C_0^\infty(\mathbb{R}^3)$ for a core, while it is not a core for $-D^2 + V$ (rather $e^{+i\lambda}(C_0^\infty)$ will be a core). Thus as regards essential self-adjointness on $C_0^\infty(\mathbb{R}^3)$, one must be prepared to change to a convenient gauge. By solving the partial differential equation $-\Delta\lambda = \operatorname{div} \mathbf{a}$, we can always find $\tilde{\mathbf{a}}$ with $\operatorname{div} \tilde{\mathbf{a}} = 0$ so that $\mathbf{a}$ and $\tilde{\mathbf{a}}$ are related by a gauge transformation.

The following theorem is proven in a reference to be found in the Notes.

Theorem X.35 Let V obey the conditions of Theorem X.29. Suppose that $\tilde{\mathbf{a}} \in L^q_{\text{loc}}(\mathbb{R}^n)$ with $q \geq 4$, $q > n$, and with $\operatorname{div} \tilde{\mathbf{a}} = 0$ (distributional sense). Then

$$-\sum_{j=1}^{n} (\partial_j - i a_j)^2 + V$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

X.5 The commutator theorem

Many of the self-adjointness techniques that we have discussed so far apply only to semibounded operators or forms. Further, the Kato–Rellich and KLMN theorems have the feature that perturbations of positive operators are semibounded. In this section we prove several theorems which are useful for proving the self-adjointness of nonsemibounded operators. At the end of the section we apply the theorem to the Stark effect Hamiltonian, i.e., the Hamiltonian of an atom in a constant electric field.

Although the operator A whose self-adjointness we wish to establish will not be semibounded, we will assume that A can be estimated in various ways by an auxiliary self-adjoint operator N that is semibounded.

Throughout this section we will assume that $N \geq I$. We will denote by $\mathscr{H}_n$, $n = 0, \pm 1, \pm 2, \ldots$, the completion of $D(N^{n/2})$ in the norm

$$\|\psi\|_n = \|N^{n/2}\psi\| \tag{X.50}$$

We thus have the scale of spaces $\cdots \mathscr{H}_n \supset \mathscr{H}_{n+1} \cdots$ discussed in the Appendix to Section IX.4 and introduced for the cases $n = 0, \pm 1$ in Section VIII.6. Recall that for $n > 0$, $\mathscr{H}_n = D(N^{n/2})$ and that $\mathscr{H}_{-n}$ can be identified with $\mathscr{H}_n^*$.

Suppose that $a(\cdot, \cdot)$ is a quadratic form on $Q(a) = D(N^{n/2})$ which satisfies

$$|a(\varphi, \psi)| \leq c\|\varphi\|_n \|\psi\|_n \tag{X.51}$$

Thus for each $\varphi \in \mathscr{H}_n$, there is a $\tilde{\varphi} \in \mathscr{H}_{-n}$ so that $a(\varphi, \psi) = \tilde{\varphi}(\psi)$ for all $\psi \in \mathscr{H}_n$. The map $\varphi \overset{A}{\mapsto} \tilde{\varphi}$ is linear and bounded so $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$. Conversely, any $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$ gives rise to a quadratic form $a(\cdot, \cdot)$ on $Q(a) = D(N^{n/2})$ satisfying (X.51). For such an A, the adjoint A^* is a bounded operator from $\mathscr{H}_{-n}^*$ to $\mathscr{H}_n^*$. But since $\mathscr{H}_{-n}^*$ and $\mathscr{H}_n^*$ are naturally isomorphic to $\mathscr{H}_n$ and $\mathscr{H}_{-n}$, A^* is in a natural way also a bounded operator from $\mathscr{H}_n$ to $\mathscr{H}_{-n}$. If $A = A^*$, then we say that $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$ is **symmetric**. Clearly, this is equivalent to saying that the corresponding form $a(\cdot, \cdot)$ is symmetric.

Given an $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$ we can define $[N, A]$ as an operator from $\mathscr{H}_{n+2}$ to $\mathscr{H}_{-n-2}$ by

$$[N, A]\psi = N(A\psi) - A(N\psi), \qquad \psi \in \mathscr{H}_{n+2} \tag{X.52}$$

Since N is bounded from $\mathscr{H}_{n+2}$ to $\mathscr{H}_n$ and from $\mathscr{H}_{-n}$ to $\mathscr{H}_{-n-2}$, $[N, A]$ is a bounded operator from $\mathscr{H}_{n+2}$ to $\mathscr{H}_{-n-2}$. If for each $\psi \in \mathscr{H}_{n+2}$, we have that $[N, A]\psi \in \mathscr{H}_{-n}$ and

$$\|[N, A]\psi\|_{-n} \leq c\|\psi\|_n \tag{X.53}$$

then $[N, A]$ extends by the B.L.T. theorem to a bounded operator from $\mathscr{H}_n$ to $\mathscr{H}_{-n}$. In this case, we denote the extension by $[N, A]$ also.

Finally, given a quadratic form $a(\cdot, \cdot)$ on $D(N^{n/2})$, or what amounts to the same thing, an $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$, we define an associated operator $\hat{A}$ on $\mathscr{H}$ by

$$D(\hat{A}) = \{\psi \in \mathscr{H} \cap \mathscr{H}_n \,|\, A\psi \in \mathscr{H}\}$$
$$\hat{A}\psi = A\psi, \qquad \psi \in D(\hat{A})$$

In general, $D(\hat{A})$ need not be dense. In fact, in Problem 34, the domain of $\hat{A}$ consists of just the zero vector.

We can now state the main theorem of this section. Later on (Theorem X.37) we will prove a related theorem with "operator" hypotheses rather than "form" hypotheses.

Theorem X.36 (the commutator theorem) Let N be a self-adjoint operator with $N \geq I$. Suppose that A is a symmetric operator in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ where $\mathscr{H}_n$ is the scale associated with N. Suppose that, in addition, $[N, A]$ is in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$. Then:

(a) The associated operator $\hat{A}$ is densely defined.
(b) $D(N) \subset D(\hat{A})$ and for all $\psi \in D(N)$,

$$\|\hat{A}\psi\| \leq c\|N\psi\| \tag{X.54}$$

(c) $\hat{A}$ is essentially self-adjoint on any core for N.

For clarity, we restate Theorem X.36 without mention of the scale $\mathscr{H}_n$:

Theorem X.36' Let N be a self-adjoint operator with $N \geq I$. Suppose that $a(\cdot, \cdot)$ is a quadratic form with $Q(a) = Q(N)$ so that:

(i) $|a(\psi, \varphi)| \leq c_1\|N^{1/2}\varphi\| \, \|N^{1/2}\psi\|$ for all $\varphi, \psi \in D(N^{1/2})$;
(ii) $|a(N\psi, \varphi) - a(\psi, N\varphi)| \leq c_2\|N^{1/2}\varphi\| \, \|N^{1/2}\psi\|$ for all $\varphi, \psi \in D(N^{3/2})$.

Then

(a, b') For any $\psi \in D(N)$ and all $\varphi \in D(N^{1/2})$,

$$|a(\varphi, \psi)| \leq c\|\varphi\| \, \|N\psi\|$$

so $\psi \in D(\hat{A})$ and $a(\varphi, \psi) = (\varphi, \hat{A}\psi)$ for all $\varphi \in D(N^{1/2})$ and $\hat{A}\psi$ satisfies (X.54).

(c) $\hat{A}$ is essentially self-adjoint on any core for N.

We begin the proof with two general lemmas about scales of spaces. We denote the norm in $\mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$ by $\|\cdot\|_{n,m}$.

Lemma 1 If $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$ and $[N, A] \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$, then

$$A \in \mathscr{L}(\mathscr{H}_{n+2}, \mathscr{H}_{m+2})$$

Proof Let $\psi \in \mathscr{H}_{n+2}$. A priori $NA\psi \in \mathscr{H}_{m-2}$, but $AN\psi \in \mathscr{H}_m$ since $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$, and $NA\psi - AN\psi \in \mathscr{H}_m$ since $[N, A] \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$. Thus $NA\psi \in \mathscr{H}_m$ and

$$\begin{aligned}\|A\psi\|_{m+2} &= \|NA\psi\|_m \\ &\leq \|[N, A]\psi\|_m + \|AN\psi\|_m \\ &\leq \|[N, A]\|_{n,m}\|\psi\|_n + \|A\|_{n,m}\|N\psi\|_n \\ &\leq (\|[N, A]\|_{n,m} + \|A\|_{n,m})\|\psi\|_{n+2}\end{aligned}$$

so $A \in \mathscr{L}(\mathscr{H}_{n+2}, \mathscr{H}_{m+2})$ and

$$\|A\|_{n+2,m+2} \leq \|[N, A]\|_{n,m} + \|A\|_{n,m} \quad \blacksquare$$

Lemma 2 If $A \in \mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ and $[N, A] \in \mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$, then $A \in \mathscr{L}(\mathscr{H}_{+2}, \mathscr{H})$, i.e., $D(\hat{A}) \supset D(N)$ and (X.54) holds.

Proof By Lemma 1, $A \in \mathscr{L}(\mathscr{H}_{+3}, \mathscr{H}_{+1})$. Interpolating between $\mathscr{L}(\mathscr{H}_{+3}, \mathscr{H}_{+1})$ and $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ (see the Appendix to Section IX.4), we conclude that $A \in \mathscr{L}(\mathscr{H}_{+2}, \mathscr{H})$. $\blacksquare$

Proof of Theorem X.36 By Lemma 2, (a) and (b) hold. Suppose we prove that $\hat{A}$ is essentially self-adjoint on $D(N)$. Let C be a core for N. By (X.54), $\overline{\hat{A} \restriction C} \supset \hat{A} \restriction D(N)$ so $\hat{A}$ is essentially self-adjoint on C and (c) follows. Thus, we need only show that $\hat{A} \restriction D(N)$ is essentially self-adjoint. Let us denote $\hat{A} \restriction D(N)$ by B and suppose $\psi \in D(B^*)$. Then $\varphi \equiv N^{-1}\psi \in D(N) \subset D(B)$. We compute

$$\begin{aligned}|\mathrm{Im}(\varphi, B^*\psi)| &= \frac{1}{2}\,|i(\varphi, B^*\psi) - i(B^*\psi, \varphi)| \\ &= \frac{1}{2}\,|i(A\varphi, N\varphi) - i(N\varphi, A\varphi)| \\ &\leq \frac{1}{2}\,\|[N, A]\|_{+1,-1}\,\|\varphi\|_{+1}^2 \\ &\leq \frac{c}{2}\,\|\varphi\|_{+1}^2 = \frac{c}{2}\,(\varphi, \psi)\end{aligned}$$

where $c \geq \|[N, A]\|_{+1,-1}$. Thus, since (φ, ψ) is real and nonnegative,

$$\mathrm{Im}(\varphi, (\pm B^* + ic)\psi) \geq \frac{c}{2}\,(\varphi, \psi)$$

Therefore, if $(B^* \mp ic)\psi = 0$, then $(\varphi, \psi) = (\psi, N^{-1}\psi) \leq 0$. Since N^{-1} is positive with zero kernel, $\psi = 0$. We have thus proven that $\mathrm{Ker}(B^* \pm ic) = 0$, so B is essentially self-adjoint by the fundamental criterion. $\blacksquare$

An important application of Theorem X.36 appears at the end of this section. We begin here with several examples showing that certain of the hypotheses cannot be weakened.

Example 1 Let $N = p^2 + q^2$ on $L^2(\mathbb{R}, dx)$ where $p = i^{-1}\, d/dx$ and let $A = p^2 + q^2 - q^4$. By application of the methods of the Appendix to Section X.1, A is not essentially self-adjoint on $C_0^\infty(\mathbb{R})$ which is a core for N. But A and $[N, A]$ lie in $\mathscr{L}(\mathscr{H}_{+2}, \mathscr{H}_{-2})$. Thus the 1 in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ is crucial for Theorem X.36. In fact, if we take $N = (p^2 + q^2)^k$ we see that $A \in \mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ if $k \geq 2$ while $[N, A] \in \mathscr{L}(\mathscr{H}_\alpha, \mathscr{H}_{-\alpha})$ with $\alpha = 1 + k^{-1}$ (using the natural object for $\mathscr{H}_\alpha$ when α is nonintegral). Thus the ± 1 in the condition on $[N, A]$ cannot be changed even a little.

Example 2 Let $H = p^2 + q^2 + q^4$ and define $q(t) = e^{iHt} q e^{-iHt}$. Since q is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$ and $q^2 \leq cH^2$, $D(q) \supset D(H) \supset \mathscr{S}(\mathbb{R})$ and q is essentially self-adjoint on $D(H)$. Since $e^{iHt}\colon D(H) \to D(H)$, each $q(t)$ is essentially self-adjoint on $D(H)$ also. But what about $q(t_1) + q(t_2)$? This is not so easy by the methods preceding Theorem X.36. But $\pm q \leq H + 1$ so q and $q(t_1) + q(t_2)$ are in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ if $N = H$. Furthermore, $\pm i[H, q] = \pm 2p \leq 2H + 2$ so $[H, q(t_1) + q(t_2)]$ lies in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ also. Thus, by Theorem X.36, $q(t_1) + q(t_2)$ is essentially self-adjoint on any core for H.

Example 3 Let $h(\varphi, \psi) = (\varphi, (p^2 + q^2 + \delta(q))\psi)$ on $\mathscr{S}(\mathbb{R}) \times \mathscr{S}(\mathbb{R})$. Since $\delta(q)$ is p^2-form small, the KLMN theorem guarantees a self-adjoint operator H corresponding to the form h. Let $p(t) = e^{iHt} p e^{-iHt}$. Since $[p, H]$ is badly behaved, we cannot control $p(t_1) + p(t_2)$ by the method of Example 2. However, for each real-valued $f \in C_0^\infty(\mathbb{R})$, define

$$a_f(\varphi, \psi) = \int f(t)(\varphi, p(t)\psi)\, dt, \qquad \varphi, \psi \in Q(H)$$

Then a_f is symmetric and

$$\begin{aligned} |a_f(\varphi, \varphi)| &\leq \int |f(t)|\, |(e^{-iHt}\varphi, pe^{-iHt}\varphi)|\, dt \\ &\leq \int |f(t)|\, |(e^{-iHt}\varphi, cHe^{-iHt}\varphi)|\, dt \\ &\leq ch(\varphi, \varphi) \int |f(t)|\, dt \\ &= c\|H^{1/2}\varphi\|^2 \|f\|_1 \end{aligned}$$

for all $\varphi \in Q(H)$. Further, for $\varphi \in D(H^2)$

$$\begin{aligned} a_f(H\varphi, \varphi) - a_f(\varphi, H\varphi) &= \int f(t)\{(H\varphi, p(t)\varphi) - (\varphi, p(t)H\varphi)\}\, dt \\ &= \int f(t) \frac{d}{dt} (\varphi, p(t)\varphi)\, dt \\ &= -\int f'(t)(\varphi, p(t)\varphi)\, dt \end{aligned}$$

Thus,

$$\begin{aligned} |a_f(H\varphi, \varphi) - a_f(\varphi, H\varphi)| &\leq ch(\varphi, \varphi)\|f'\|_1 \\ &\leq c\|H^{1/2}\varphi\|^2\|f'\|_1 \end{aligned}$$

So, by Theorem X.36′, there is a self-adjoint operator A_f associated to the quadratic form a_f and A_f is self-adjoint on any core for H. *Formally*, A_f is just $\int_{-\infty}^{\infty} f(t)p(t)\, dt$. Of course, the particular operator we have considered is not very important. What we have illustrated is that if we only know that $\pm B \leq cH$, then we can prove essential self-adjointness for

$$B_f = \int f(t)e^{iHt}Be^{-iHt}\, dt$$

for real-valued $f \in C_0^\infty(\mathbb{R})$. Such a situation arises in quantum field theory (see the references in the Notes).

Example 4 There is a connection between Theorem X.36 and a technique in the theory of ordinary differential equations. We will illustrate the technique in a case which is also easy to handle by other means. Suppose that we want to solve

$$\ddot{q}(t) = F(q(t)) \tag{X.55}$$

for a real-valued function $q(t)$ where F is some Lipschitz function obeying

$$|F(x)| \leq |x| \tag{X.56}$$

It is easy to prove local solvability of (X.55) given initial conditions (see Section V.6). To prove global solvability, we let $p = \dot{q}$ so that (X.55) becomes

$$\dot{q}(t) = p(t) \tag{X.57a}$$

$$\dot{p}(t) = F(q(t)) \tag{X.57b}$$

Let $N(p, q) = p^2 + q^2$ and let $N(t) = N(p(t), q(t))$. Suppose that we can show that for any solution on $[0, t_0)$, $N(t)$ stays bounded as $t \to t_0$. Then by a maximum interval argument similar to that used in the proof of Proposition 1 in the Appendix to X.1, we can extend the solution to $t_0 + \varepsilon$. In this way one proves that global solutions exist. To prove that $N(t)$ is bounded, we show that

$$\dot{N}(t) \leq 2N(t) \tag{X.58}$$

For

$$\begin{aligned}\dot{N}(t) &= 2pF(q) + 2pq \\ &\leq 4|pq| \leq 2N(t)\end{aligned}$$

by (X.57) and (X.56). By integrating (X.58) we see that

$$N(t) \leq N(0)e^{2t}$$

Let us consider a formal proof of a part of Theorem X.36 based on these classical ideas. Suppose that A, N obey the hypotheses of the theorem and let $\tilde{A}$ be a self-adjoint extension, if such exists. Let $\psi \in Q(N)$ and let

$$N(t) = (\psi, e^{i\tilde{A}t}Ne^{-i\tilde{A}t}\psi)$$

Then *formally*

$$\begin{aligned}\dot{N}(t) &= (e^{-i\tilde{A}t}\psi, i[A, N]e^{-i\tilde{A}t}\psi) \\ &\leq cN(t)\end{aligned}$$

by the bound on $i[A, N]$. This suggests that $e^{-i\tilde{A}t}$ leaves $Q(N)$ invariant which is the beginning of the self-adjointness proof of Theorem VIII.10. These formal ideas can be turned into a proof of a slightly weakened form of Theorem X.36 (see the reference in the Notes).

For our discussion of the Stark effect we need an alternative version of Theorem X.36. As it stands we need information about $D(N^{3/2})$ or $D(N^k)$ for $k \geq \frac{3}{2}$. If N is not a simple operator, it may even be very difficult to determine a core for $D(N^k)$ if $k > 1$. In such a situation the following theorem with "operator" hypotheses is useful.

Theorem X.37 Let N be a self-adjoint operator with $N \geq 1$. Let A be a symmetric *operator* with domain D which is a core for N. Suppose that:

(i) For some c and all $\varphi \in D$,

$$\|A\varphi\| \leq c\|N\varphi\| \tag{X.59}$$

(ii) For some d and all $\varphi \in D$,

$$|(A\varphi, N\varphi) - (N\varphi, A\varphi)| \leq d\|N^{1/2}\varphi\|^2 \tag{X.60}$$

Then A is essentially self-adjoint on D and its closure is essentially self-adjoint on any other core for N.

Proof By (i), the closure of A has a domain containing $D(N)$ and (ii) extends to all $\varphi \in D(N)$. By mimicking the proof of Theorem X.36 one shows that $\mathrm{Ker}(A^* \pm id) = \{0\}$ and thus A is essentially self-adjoint. ∎

We remark on one vaguely annoying feature of Theorem X.37. Namely, we need to suppose that A is an N-bounded operator and not merely an N-bounded form as in Theorem X.36. At first sight this is surprising since Lemma 2 above seems to imply that condition (ii) of Theorem X.37 and the weaker:

(i′) For some c and all $\varphi \in D$,

$$|(\varphi, A\varphi)| \leq c(\varphi, N\varphi)$$

should imply (i). The fallacy in this is that (ii) is slightly different from condition (ii) of Theorem X.36′. To have the latter we would need (X.60) for a set of φ which includes a core for $N^{3/2}$. A priori, D might be disjoint from $D(N^{3/2})$. To tantalize us, (i) implies that (ii) extends to all φ in $D(N)$ and so to $D(N^{3/2})$, but (i′) does not; so it seems impossible to use (i′) and (ii). In any event, we will need a separate argument to prove (X.59) in the following application:

Theorem X.38 (the Faris–Lavine theorem) Let V and W be real-valued measurable functions on $\mathbb{R}^n$ with

$$V(x) \geq -cx^2 - d$$

$V \in L^2_{\mathrm{loc}}(\mathbb{R}^n)$ and suppose that:

(i) There exists a dense set $D \subset D(-\Delta) \cap D(V) \cap D(W)$ which is left invariant by x_j and $i^{-1}\,\partial/\partial x_j$ so that $-\Delta + V + W + 2cx^2$ is essentially self-adjoint on D.

(ii) For some $a < 1$, $-a\Delta + W$ is bounded from below on D.

Then $-\Delta + V + W$ is essentially self-adjoint on D.

Proof By (ii) and the hypotheses on V, we can choose b so that

$$N = -\Delta + V + W + 2cx^2 + b \geq 1$$

Let $A = -\Delta + V + W$. We will verify (X.59) and (X.60) on D. As quadratic forms on D:

$$N^2 = (A + b + 2cx^2)^2 = (A + b)^2 + 4c^2x^4 + 2c(Ax^2 + x^2A) + 4bcx^2$$

$$= (A + b)^2 + 4c^2x^4 + 4c\sum_{j=1}^{n} x_j(A + b)x_j + 2c\sum_j [x_j, [x_j, A]]$$

$$= (A + b)^2 + 4c\sum_{j=1}^{n} x_j(A + b + cx^2)x_j - 4cn$$

By changing b if necessary, we can be sure that $A + b + cx^2 \geq 0$ so that

$$\|(A + b)\psi\|^2 \leq \|N\psi\|^2 + 4cn\|\psi\|^2$$

proving (X.59).

Similarly, in the sense of (X.60):

$$\pm i[A, N] = \pm i[A - N, N] = \pm i[-2cx^2, \Delta]$$
$$= \mp i4c(\mathbf{x} \cdot \nabla + \nabla \cdot \mathbf{x}) \leq 4c(-\Delta + x^2)$$
$$\leq dN$$

where we have used

$$-\Delta + x^2 \mp i(\mathbf{x} \cdot \nabla + \nabla \cdot \mathbf{x}) = (i\nabla \mp \mathbf{x})^2 \geq 0$$

and the fact that

$$N = (-a\Delta + W) + (V + cx^2) + (1 - a)(-\Delta) + cx^2$$
$$\geq e(-\Delta + x^2) - f$$

Thus by Theorem X.37, A is essentially self-adjoint on D. ∎

Corollary Let real-valued measurable functions V_1 and V_2 be given which satisfy:

(i) $V_2 \in L^p(\mathbb{R}^n)$ with $p \geq 2$ if $n \leq 3$, $p > 2$ if $n = 4$, and $p \geq n/2$ if $n \geq 5$.
(ii) $V_1 \geq -cx^2 - d$ for some c and d; $V_1 \in (L^2)_{\text{loc}}$.

Then $-\Delta + V_1 + V_2$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Proof Let $V = -cx^2 - d$ and $W = V_1 + V_2 + cx^2 + d$. Then by Theorem X.29, $-\Delta + W + V + 2cx^2$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ since V_2 is $-\Delta$-bounded and $V_1 + 2cx^2 + d$ is positive. Further, $-a\Delta + W$ is bounded below for any $a > 0$. Thus, by Theorem X.38, $-\Delta + V + W$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. ∎

Similarly, combining Theorem X.30, Theorem X.38, and the uncertainty principle lemma we have:

Corollary If $V(\mathbf{r}) \geq \frac{1}{4}n(4-n)r^{-2} - cr^2 - d$, then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \backslash \{0\})$.

Example 5 (the Stark effect) The Hamiltonian of an atom in a constant electric field $\mathbf{E}_0$ is

$$H = -\sum_{n=1}^{N} (2m)^{-1}\Delta_n - (2M)^{-1}\Delta_0 - \sum_{n=1}^{N} \frac{Ne^2}{|\mathbf{x}_n - \mathbf{x}_0|} + \frac{1}{2}\sum_{n \neq m} \frac{e^2}{|\mathbf{x}_n - \mathbf{x}_m|}$$
$$+ e\mathbf{E}_0 \cdot \left(\mathbf{x}_0 - \sum_{n=1}^{N} \mathbf{x}_n\right)$$

By the first corollary, H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3N+3})$.

By the above method one can also treat simultaneous electric and magnetic fields (see Problem 38).

X.6 Analytic vectors

Stone's theorem says that there is a one-to-one correspondence between self-adjoint operators and continuous one-parameter unitary groups. This suggests that if a symmetric operator A "determines" a unique group, then A should be essentially self-adjoint. In fact, Theorem VIII.10 says that if $U(t)$ is a continuous one-parameter unitary group, $U(t)$: $D(A) \to D(A)$ and $U'(t)\varphi = iAU(t)\varphi$ for $\varphi \in D(A)$, then A is essentially self-adjoint and generates $U(t)$. We are looking for conditions on a symmetric operator that guarantee that such a group can be constructed. The most natural way to construct $U(t)$ is to try to make sense of the power series $\sum_{n=0}^{\infty} (itA)^n/n!$ on a dense set of vectors. Notice that this can certainly be done if A is self-adjoint. For let E_Ω be the family of spectral projections for A. Then on each of the spaces $E_{[-M,M]}$, A is a bounded operator and $\sum_{n=0}^{\infty} (itA)^n/n!$ converges to e^{itA} in norm. In particular, for any $\varphi \in \bigcup_{M \geq 0} E_{[-M,M]}$,

$$\sum_{n=0}^{N} \frac{(itA)^n}{n!}\varphi \to e^{itA}\varphi$$

Since $\bigcup_{M\geq 0} E_{[-M,M]}$ is dense in $\mathscr{H}$, we see that the group generated by a self-adjoint operator A is completely determined by the well-defined action of the series $\sum_{n=0}^{\infty} (itA)^n/n!$ on a dense set. We will prove the converse: namely, if A is symmetric and has a dense set of vectors to which $\sum_{n=0}^{\infty} (itA)^n/n!$ can be applied, then A is essentially self-adjoint. We need several definitions.

Definition Let A be an operator on a Hilbert space $\mathscr{H}$. The set $C^\infty(A) \equiv \bigcap_{n=1}^{\infty} D(A^n)$ is called the **C^∞-vectors for A**. A vector $\varphi \in C^\infty(A)$ is called an **analytic vector for A** if

$$\sum_{n=0}^{\infty} \frac{\|A^n\varphi\|}{n!} t^n < \infty$$

for some $t > 0$.

If A is self-adjoint, then $C^\infty(A)$ will be dense in $D(A)$. However, in general, a symmetric operator may have no C^∞ vectors at all even if A is essentially self-adjoint. We caution the reader to remember that analytic vectors and vectors of uniqueness (defined below) must be C^∞ vectors for A. A vector $\psi \in D(A)$ can be an analytic vector for an extension of A but fail to be an analytic vector for A because it is not in $C^\infty(A)$.

Definition Suppose that A is symmetric. For each $\varphi \in C^\infty(A)$, define

$$D_\varphi = \left\{ \sum_{n=0}^{N} \alpha_n A^n \varphi \,\middle|\, N = 1, 2, \ldots, \langle \alpha_1, \ldots, \alpha_N \rangle \text{ arbitrary} \right\}$$

Let $\mathscr{H}_\varphi = \overline{D}_\varphi$ and define $A_\varphi : D_\varphi \to D_\varphi$ by $A_\varphi(\sum_{n=0}^{N} \alpha_n A^n\varphi) = \sum_{n=0}^{N} \alpha_n A^{n+1}\varphi$. φ is called a **vector of uniqueness** if and only if A_φ is essentially self-adjoint on D_φ (as an operator on $\mathscr{H}_\varphi$).

Finally, a subset S of $\mathscr{H}$ is called **total** if the set of finite linear combinations of elements of S is dense in $\mathscr{H}$.

Lemma (Nussbaum) Let A be a symmetric operator and suppose that $D(A)$ contains a total set of vectors of uniqueness. Then A is essentially self-adjoint.

Proof We will show that $\mathrm{Ran}(A \pm i)$ are dense in $\mathscr{H}$. By the fundamental criterion this will show that A is essentially self-adjoint. Suppose $\psi \in \mathscr{H}$ and $\varepsilon > 0$ are given and let S denote the set of vectors of uniqueness. Since S is total we can find $\langle \alpha_1, \ldots, \alpha_N \rangle$ and $\langle \psi_1, \ldots, \psi_N \rangle$ with $\psi_n \in S$ so

that $\|\psi - \sum_{n=1}^{N} \alpha_n \psi_n\| \leq \varepsilon/2$. Since ψ_n is a vector of uniqueness, there is a $\varphi_n \in D_{\psi_n}$ so that

$$\|\psi_n - (A + i)\varphi_n\| \leq \frac{\varepsilon}{2}\left(\sum_{n=1}^{N} |\alpha_n|\right)^{-1}$$

Setting $\varphi = \sum_{n=1}^{N} \alpha_n \varphi_n$, we have $\varphi \in D(A)$ and $\|\psi - (A + i)\varphi\| \leq \varepsilon$. Thus $\mathrm{Ran}(A + i)$ is dense. The proof for $(A - i)$ is the same. ∎

Theorem X.39 (Nelson's analytic vector theorem) Let A be a symmetric operator on a Hilbert space $\mathscr{H}$. If $D(A)$ contains a total set of analytic vectors, then A is essentially self-adjoint.

Proof By Nussbaum's lemma, it is enough to show that each analytic vector ψ is a vector of uniqueness. First notice that by Theorem X.3, A_ψ always has self-adjoint extensions, since the operator

$$C: \sum_{n=0}^{N} \alpha_n A^n \psi \to \sum_{n=0}^{N} \bar{\alpha}_n A^n \psi$$

extends to a conjugation on $\mathscr{H}_\psi$ which commutes with A_ψ. Suppose that B is a self-adjoint extension of A_ψ on $\mathscr{H}_\psi$ and let μ be the spectral measure for B associated to ψ. Since ψ is an analytic vector for A, $\sum_{n=0}^{\infty} (\|A^n\psi\|/n!)t^n < \infty$ for some $t > 0$. Let $0 < s < t$. Then

$$\sum_{n=0}^{\infty} \frac{s^n}{n!} \int_{-\infty}^{\infty} |x|^n \, d\mu \leq \sum_{n=0}^{\infty} \frac{s^n}{n!} \left(\int_{-\infty}^{\infty} x^{2n} \, d\mu\right)^{1/2} \left(\int_{-\infty}^{\infty} d\mu\right)^{1/2}$$

$$= \|\psi\| \sum_{n=0}^{\infty} \frac{s^n}{n!} \|A^n\psi\| < \infty$$

Thus, by Fubini's theorem,

$$\int_{-\infty}^{\infty} \sum_{n=0}^{\infty} \frac{s^n}{n!} |x|^n \, d\mu = \int_{-\infty}^{\infty} e^{s|x|} \, d\mu < \infty$$

As a result, the function $(\psi, e^{itB}\psi) = \int_{-\infty}^{\infty} e^{itx} \, d\mu$ has an analytic continuation $\int_{-\infty}^{\infty} e^{izx} \, d\mu$ to the region $|\mathrm{Im}\, z| < t$. Since

$$\left[\left(\frac{d}{dz}\right)^k \int_{-\infty}^{\infty} e^{izx} \, d\mu\right]_{z=0} = \int_{-\infty}^{\infty} (ix)^k \, d\mu = (\psi, (iA)^k\psi)$$

we have

$$(\psi, e^{isB}\psi) = \sum_{n=0}^{\infty} \frac{(is)^n}{n!} (\psi, A^n\psi)$$

for $|s| < t$. Thus, for $|s| < t$ (and therefore for all s), the function $(\psi, e^{isB}\psi)$ is completely determined by the numbers $(\psi, A^n\psi)$, $n = 0, 1, 2, \ldots$. A

similar proof shows that $(\psi_1, e^{isB}\psi_2)$ is determined by the numbers $(\psi_1, A^n\psi_2)$, $n = 0, 1, 2, \ldots$, for any $\psi_1, \psi_2 \in D_\psi$. Since D_ψ is dense in $\mathscr{H}_\psi$ and e^{isB} is unitary, e^{isB} is completely determined by the numbers $(\psi_1, A^n\psi_2)$ for $\psi_1, \psi_2 \in D_\psi$ and $n = 0, 1, 2, \ldots$. Thus, all self-adjoint extensions of A_ψ generate the same unitary group, so by Stone's theorem A_ψ has at most one self-adjoint extension. As we have already remarked, A_ψ has at least one self-adjoint extension. Thus A_ψ is essentially self-adjoint and ψ is a vector of uniqueness. ∎

Corollary 1 A closed symmetric operator A is self-adjoint if and only if $D(A)$ contains a dense set of analytic vectors.

The statement of Corollary 1 is not true if "self-adjoint" is replaced by "essentially self-adjoint." A self-adjoint operator A may be essentially self-adjoint on a domain $D \subset D(A)$ and D may not even contain any C^∞ vectors. The reader is asked to construct an example in Problem 39.

Corollary 2 Suppose that A is a symmetric operator and let D be a dense linear set contained in $D(A)$. Then, if D contains a dense set of analytic vectors *and if* D *is invariant under* A, then A is essentially self-adjoint on D.

Proof Since D is invariant under A, each analytic vector for A in D is also an analytic vector for $A \restriction D$. Thus, by Theorem X.39 $A \restriction D$ is essentially self-adjoint. ∎

The reason that one needs the invariance condition in Corollary 2 is that for a vector $\psi \in D$ to be analytic for $A \restriction D$, it must first be C^∞ for $A \restriction D$. This requires that $A^n\psi \in D$ for all n. The following is a simple example which shows why one must be very careful of this invariance condition.

Example 1 Let $\mathscr{H} = \ell_2$ and let A be the self-adjoint operator which has the vectors $\delta_n = \langle 0, 0, \ldots, 1, 0, 0, \ldots \rangle$ as eigenfunctions with $A\delta_n = n\delta_n$. By Proposition 1 of Section VIII.3, $D(A) = \{\{a_n\} \mid \{na_n\} \in \ell_2\}$. Now, let $D = \{\sum_{n=1}^N \alpha_n \delta_n \mid \sum \alpha_n = 0, N \text{ arbitrary but finite}\}$. First, it is clear that each vector in D is an analytic vector for A, since $\|A^k \sum_{n=1}^N \alpha_n \delta_n\|^2 \leq N^{2k} \sum_{n=1}^N |\alpha_n|^2$. Secondly, D is dense in ℓ_2. For, suppose that $\{a_n\}$ is a sequence in ℓ_2 which is zero after the Mth place. Then the vector

$$\varphi = \Big\langle a_1, \ldots, a_M, \underbrace{\frac{-\sum_{i=1}^M a_i}{k}, \ldots, \frac{-\sum_{i=1}^M a_i}{k}}_{k \text{ places}}, 0, \ldots \Big\rangle$$

is in D and satisfies

$$\|\{a_n\} - \varphi\|_{\ell_2} \leq \left| \sum_{i=1}^{N} a_i \right| k^{-1/2}$$

Thus $\{a_n\}$ can be approximated by elements of D. Since the set of such $\{a_n\}$ are dense, so is D.

Thus, D is a dense set of analytic vectors for A, But, $A \restriction D$ is *not* essentially self-adjoint. For, let $\psi = \{1/n\}_{n=1}^{\infty}$. Then, for all $\varphi \in D$, $(A\varphi, \psi) = 0$. So, $\psi \in D((A \restriction D)^*)$ and $(A \restriction D)^*\psi = 0$. This shows that $D((N \restriction D)^*)$ *strictly* contains $D(A)$, so A is not essentially self-adjoint on D. Notice, that A does not take D into itself.

The following examples illustrate in a simple way how analytic vectors can be used. Some applications of analytic vectors in quantum field theory are described in the next section.

Example 2 Let A and $A^\dagger$ be the maps of $\mathscr{S}(R)$ into itself given by

$$A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right), \qquad A^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)$$

and define $N = A^\dagger A$. Let $\phi_0 = \pi^{-1/4}e^{-x^2/2}$ and $\phi_n = (n!)^{-1/2}(A^\dagger)^n\phi_0$. The ϕ_n are just the Hermite functions which form an orthonormal basis for $L^2(\mathbb{R})$ (see Problems 6 and 7 of Chapter IX). The operator N satisfies $N\phi_n = n\phi_n$ and A and $A^\dagger$ satisfy the commutation relation (on $\mathscr{S}(\mathbb{R})$):

$$AA^\dagger - A^\dagger A = I$$

It follows easily that $A^\dagger\phi_n = \sqrt{n+1}\,\phi_{n+1}$ and $A\phi_n = \sqrt{n}\,\phi_{n-1}$ if $n \geq 1$, and $A\phi_0 = 0$. Therefore

$$\|\underbrace{A^\# A^\# \cdots A^\#}_{k \text{ times}}\phi_n\| \leq (n+1)^{1/2} \cdots (n+k)^{1/2} \leq [(n+k)!]^{1/2} \quad \text{(X.61)}$$

where each $A^\#$ can represent either A or $A^\dagger$. Since $x^k = 2^{-k/2}(A + A^\dagger)^k$, (X.61) implies

$$\|x^k\phi_n\| \leq 2^{k/2}[(n+k)!]^{1/2}$$

and therefore

$$\sum_{k=0}^{\infty} \frac{\|x^k\phi_n\|}{k!} t^k \leq \sum_{k=0}^{\infty} \frac{2^{k/2}[(n+k)!]^{1/2}}{k!} t^k < \infty$$

for all t so each ϕ_n is an analytic vector for x. Since the set of finite linear combinations of the Hermite functions is a dense set invariant under x, we conclude that x is essentially self-adjoint on any linear subspace of $L^2(\mathbb{R})$ contained in $\{\varphi \mid \|x\varphi\|_2 < \infty\}$ which contains the Hermite functions. A similar statement holds for $i\,d/dx$.

Example 3 Let A_n be a self-adjoint operator on $\mathscr{H}_n$, $n = 1, 2, \ldots, N$, and suppose that $P(x_1, \ldots, x_N)$ is a polynomial with real coefficients of degree n_k in x_k. Let D_k^e be a domain of essential self-adjointness for A_k. Under these hypotheses, we proved in Theorem VIII.33 that the operator $P(A_1, \ldots, A_N)$ on $\mathscr{H}_1 \otimes \cdots \otimes \mathscr{H}_N$ is essentially self-adjoint on

$$D^e = \bigotimes_{n=1}^{N} D_n^e$$

The proof given in Theorem VIII.33 depended on the spectral theorem. Here we will give another proof which uses analytic vectors. $P(A_1, \ldots, A_N)$ is clearly symmetric on $D^e = \bigotimes_{n=1}^N D_k^e$. Further, since $\overline{A_n \restriction D_n^e} = A_n$, the closure of $P(A_1, \ldots, A_N)$ on D^e is the same as the closure of $P(A_1, \ldots, A_N)$ on $D = \bigotimes_{n=1}^N D(A_k)$. Therefore, it suffices to prove that $P(A_1, \ldots, A_N)$ is essentially self-adjoint on D. Let E_Ω^n be the projection-valued measure of A_n and suppose that M_n, $n = 1, \ldots, N$, are nonnegative numbers. Let $\varphi_n \in E^n_{[-M_n, M_n]}\mathscr{H}_n$; then $\|A_n\varphi_n\| \leq M_n\|\varphi_n\|$ and if $\varphi = \varphi_1 \otimes \cdots \otimes \varphi_N$ a short calculation shows that

$$\|[P(A_1, \ldots, A_N)]^k\varphi\| \leq (\tilde{P}(M_1, \ldots, M_N))^k\|\varphi\|$$

where the $\tilde{P}$ is the same polynomial as P except that each coefficient has been replaced by its absolute value. This implies that

$$\sum_{k=0}^{\infty} \frac{\|P(A_1, \ldots, A_N)^k\varphi\|}{k!}\, t^k < \infty$$

for all t so φ is an analytic vector for $P(A_1, \ldots, A_N)$. The set of finite linear combinations of such vectors is invariant under $P(A_1, \ldots, A_N)$ and is a dense subset of D. Thus, by Nelson's theorem, $P(A_1, \ldots, A_N)$ is essentially self-adjoint on D and therefore also on D^e (as remarked above).

Example 4 (Hamburger moment problem—uniqueness) In Example 3 of Section X.1 we proved a theorem giving necessary and sufficient conditions on a sequence of real numbers so that $a_n = \int_{\mathbb{R}} x^k\, d\rho(x)$ for some positive measure ρ. We will use the notation of that example. Suppose that there exist constants C and D so that $|a_n| \leq CD^n n!$ for all n. Since $\hat{A}$: $P/Q \to P/Q$,

each vector in P/Q is a C^∞ vector for $\hat{A}$. The bounds on $\{a_n\}$ thus immediately imply that P/Q is a dense set of analytic vectors for $\hat{A}$. By Theorem X.39, $\hat{A}$ is essentially self-adjoint on P/Q and thus $\hat{A} = \tilde{A}$.

Therefore $\hat{A}$ and thus the measure ρ are uniquely determined by the sequence $\{a_n\}$. Thus in the case where $|a_n| \leq CD^n n!$, we have proven that the Hamburger moment problem has a unique solution.

Various extensions of Nelson's theorem are discussed in the Notes. The reader can prove (Problem 42) the following extension in the semibounded case by using methods similar to those used above.

Definition Let A be an operator on a Hilbert space $\mathscr{H}$. A vector $\varphi \in C^\infty(A)$ is called a **semianalytic** vector for A if

$$\sum_{n=0}^{\infty} \frac{\|A^n \varphi\|}{(2n)!} t^n < \infty$$

for some $t > 0$.

Theorem X.40 Let A be a *semibounded* symmetric operator. If $D(A)$ contains a total set of semianalytic vectors, then A is essentially self-adjoint.

Theorem X.40 has two corollaries analogous to the corollaries of Theorem X.39.

Example 5 (essential self-adjointness of $H = \frac{1}{2}(-d^2/dx^2 + x^2) + x^4/4$; third proof) In terms of the notation introduced in Example 2, $H = A^\dagger A + (A^\dagger + A)^4$. Let ϕ_n be the nth Hermite function. H^k has 17^k terms each of them a product of less than or equal to $4k$ operators $A^\dagger$ or A. Thus, using (X.61) we have

$$\begin{aligned} \|H^k \phi_n\| &\leq 17^k (n+1)^{1/2} \cdots (n+4k)^{1/2} \\ &\leq 17^k 2^{2k} (2k)^{2k} c_n \end{aligned}$$

Thus, the Hermite functions are a total set of semianalytic vectors for H with domain $\mathscr{S}(\mathbb{R})$. Therefore, by Theorem X.40, H is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$, since H is clearly nonnegative.

Example 6 Using Theorem X.40 one can prove, similarly to Example 4, that the Stieltjes moment problem has a unique solution if $|a_n| \leq CD^n(2n)!$ for some constants C and D. See Problem 25.

X.7 Free quantum fields

First quantization is a mystery, but second quantization is a functor. *E. Nelson*

In Section IX.8, we described the Wightman axioms for a single scalar quantum field. In this section, we continue our discussion of quantum field theory. First, we introduce the abstract free field and use it to construct explicitly a family of examples satisfying the Wightman axioms: for each $m > 0$, we construct the free scalar field of mass m. These theories are inequivalent in the sense that there does not exist a unitary map from one Hilbert space to the other which preserves all the field theory structures (vacuum, fields, etc.). A stronger sense in which these theories are inequivalent is that the time-zero fields give different representations of the canonical commutation relations (see the Appendix to this section). In addition to proving that the axioms are satisfied, we will show that the fields are self-adjoint. The main tool in this self-adjointness proof is the analytic vector theorem.

As the name suggests, the free scalar field theories describe noninteracting particles. Nevertheless, they are important since they show that the Wightman axioms are consistent and because the most natural way to construct "interacting" theories is to make perturbations of the free theories. In the second part of this section we begin our discussion of the simplest interacting theory, the φ^4 self-interaction in two-dimensional space-time. We introduce the spatially cut-off Hamiltonian $H(g)$ and show that it is a symmetric operator. Finally, we introduce Q-space, a reformulation of the Fock space structures, which we use in Section X.9 where we prove that $H(g)$ is self-adjoint. We will *not* conclude the construction of these interacting field theories to the point of removing the spatial cut-off and proving the Wightman axioms. This has been done for a class of models; see the references in the Notes.

Let $\mathscr{H}$ be a complex Hilbert space and let $\mathscr{F}(\mathscr{H}) = \bigoplus_{n=0}^{\infty} \mathscr{H}^{(n)}$ (where $\mathscr{H}^{(n)} = \bigotimes_{k=1}^{n} \mathscr{H}$) be the Fock space over $\mathscr{H}$ defined in Section II.4. Our goal is to define the abstract free field on $\mathscr{F}_s(\mathscr{H})$, the Boson subspace of $\mathscr{F}(\mathscr{H})$; to do this we need to introduce several other families of operators and some terminology. Let $f \in \mathscr{H}$ be fixed. For vectors in $\mathscr{H}^{(n)}$ of the form $\eta = \psi_1 \otimes \cdots \otimes \psi_n$ we define a map $b^-(f)$: $\mathscr{H}^{(n)} \to \mathscr{H}^{(n-1)}$ by

$$b^-(f)\eta = (f, \psi_1)(\psi_2 \otimes \cdots \otimes \psi_n)$$

$b^-(f)$ extends by linearity to finite linear combinations of such η, the extension is well defined, and $\|b^-(f)\eta\| \leq \|f\| \, \|\eta\|$. Thus $b^-(f)$ extends to a bounded map (of norm $\|f\|$) of $\mathscr{H}^{(n)}$ into $\mathscr{H}^{(n-1)}$. Since this is true

for each n (except for $n = 0$ in which case we define $b^-(f)$: $\mathscr{H}^{(0)} \to 0$), $b^-(f)$ is in a natural way a bounded operator of norm $\|f\|$ from $\mathscr{F}(\mathscr{H})$ to $\mathscr{F}(\mathscr{H})$. It is easy to check that $b^+(f) \equiv (b^-(f))^*$ takes each $\mathscr{H}^{(n)}$ into $\mathscr{H}^{(n+1)}$ with the action

$$b^+(f)(\psi_1 \otimes \cdots \otimes \psi_n) = f \otimes \psi_1 \otimes \cdots \otimes \psi_n$$

on product vectors. Notice that the map $f \mapsto b^+(f)$ is linear, but $f \mapsto b^-(f)$ is antilinear.

Let S_n be the symmetrization operators introduced in Section II.4. Then $S = \oplus_{n=0}^{\infty} S_n$ is the projection onto the symmetric Fock space $\mathscr{F}_s(\mathscr{H}) \equiv \oplus_{n=0}^{\infty} S_n \mathscr{H}^{(n)}$. We will write $S_n \mathscr{H}^{(n)} \equiv \mathscr{H}_s^{(n)}$ and call $\mathscr{H}_s^{(n)}$ the **n-particle subspace of** $\mathscr{F}_s(\mathscr{H})$. Notice that $b^-(f)$ takes $\mathscr{F}_s(\mathscr{H})$ into itself, but that $b^+(f)$ does not. A vector $\psi = \{\psi^{(n)}\}_{n=0}^{\infty} \in \mathscr{F}_s(\mathscr{H})$ for which $\psi^{(n)} = 0$ for all but finitely many n is called a **finite particle vector**. We will denote the set of finite particle vectors by F_0. The vector $\Omega_0 = \langle 1, 0, 0, \ldots \rangle$ plays a special role; it is called the **vacuum**.

Let A be any self-adjoint operator on $\mathscr{H}$ with domain of essential self-adjointness D. Let $D_A = \{\psi \in F_0 \,|\, \psi^{(n)} \in \otimes_{k=1}^{n} D \text{ for each } n\}$ and define $d\Gamma(A)$ on $D_A \cap \mathscr{H}_s^{(n)}$ as

$$A \otimes I \otimes \cdots \otimes I + I \otimes A \otimes \cdots \otimes I + \cdots + I \otimes \cdots \otimes I \otimes A$$

In Section VIII.10, we proved that $d\Gamma(A)$ is essentially self-adjoint on D_A; $d\Gamma(A)$ is called the **second quantization** of A. For example, let $A = I$. Then its second quantization $N = d\Gamma(I)$ is essentially self-adjoint on F_0 and for $\psi \in \mathscr{H}_s^{(n)}$, $N\psi = n\psi$. N is called the **number operator**. If U is a unitary operator on $\mathscr{H}$, we define $\Gamma(U)$ to be the unitary operator on $\mathscr{F}_s(\mathscr{H})$ which equals $\otimes_{k=1}^{n} U$ when restricted to $\mathscr{H}_s^{(n)}$ for $n > 0$, and which equals the identity on $\mathscr{H}_s^{(0)}$. If e^{itA} is a continuous unitary group on $\mathscr{H}$, then $\Gamma(e^{itA})$ is the group generated by $d\Gamma(A)$, i.e., $\Gamma(e^{itA}) = e^{itd\Gamma(A)}$.

We now define the **annihilation operator** $a^-(f)$ on $\mathscr{F}_s(\mathscr{H})$ with domain F_0 by

$$a^-(f) = \sqrt{N+1}\, b^-(f) \tag{X.62}$$

$a^-(f)$ is called an annihilation operator because it takes each $(n+1)$-particle subspace into the n-particle subspace. For each ψ and η in F_0,

$$(\sqrt{N+1}\, b^-(f)\psi, \eta) = (\psi, Sb^+(f)\sqrt{N+1}\,\eta)$$

This implies that

$$(a^-(f))^* \restriction F_0 = Sb^+(f)\sqrt{N+1} \tag{X.63}$$

The operator $(a^-(f))^*$ is called a **creation operator**. Both $a^-(f)$ and $a^-(f)^* \restriction F_0$ are closable; we denote their closures by $a^-(f)$ and $a^-(f)^*$ also.

Example 1 If $\mathscr{H} = L^2(M, d\mu)$, we have seen in Section II.4 that

$$\bigotimes_{j=1}^{n} L^2(M, d\mu) = L^2(M \times \cdots \times M, d\mu \otimes \cdots \otimes d\mu)$$

and that

$$S \bigotimes_{j=1}^{n} L^2(M, d\mu) = L^2_S(M \times \cdots \times M, d\mu \otimes \cdots \otimes d\mu)$$

where L^2_S is the set of functions in L^2 which are invariant under permutations of the coordinates. The operators $a^-(f)$ and $a^-(f)^*$ are given by

$$(a^-(f)\psi)^{(n)}(m_1, \ldots, m_n) = \sqrt{n+1} \int_M \bar{f}(m)\psi^{(n+1)}(m, m_1, \ldots, m_n)\, d\mu(m)$$

$$(a^-(f)^*\psi)^{(n)}(m_1, \ldots, m_n) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} f(m_i)\psi^{(n-1)}(m_1, \ldots, \hat{m}_i, \ldots, m_n)$$

where $\hat{m}_i$ means that m_i is omitted. If A operates on $L^2(M, d\mu)$ by multiplication by the real-valued function $\omega(m)$, then

$$(d\Gamma(A)\psi)^{(n)}(m_1, \ldots, m_n) = \left(\sum_{i=1}^{n} \omega(m_i)\right)\psi^{(n)}(m_1, \ldots, m_n)$$

(X.63) implies that the **Segal field operator** $\Phi_S(f)$ on F_0 defined by

$$\Phi_S(f) = \frac{1}{\sqrt{2}}(a^-(f) + a^-(f)^*)$$

is symmetric. In fact, we will shortly see that $\Phi_S(f)$ is essentially self-adjoint. The mapping from $\mathscr{H}$ to the self-adjoint operators on $\mathscr{F}_s(\mathscr{H})$ given by

$$f \mapsto \Phi_S(f)$$

is called the **Segal quantization over** $\mathscr{H}$. Notice that the Segal quantization is a real (*but not complex*) linear map since $f \mapsto a^-(f)$ is antilinear and $f \mapsto (a^-(f))^*$ is linear. The following theorem gives the fundamental properties of the Segal quantization.

Theorem X.41 Let $\mathscr{H}$ be a complex Hilbert space; $\Phi_S(\cdot)$ the corresponding Segal quantization. Then:

(a) (self-adjointness) For each $f \in \mathscr{H}$, $\Phi_S(f)$ is essentially self-adjoint on F_0, the finite particle vectors.

(b) (cyclicity of the vacuum) Ω_0 is in the domain of all finite products $\Phi_S(f_1)\cdots\Phi_S(f_n)$ and the set $\{\Phi_S(f_1)\cdots\Phi_S(f_n)\Omega_0 \mid f_i \text{ and } n \text{ arbitrary}\}$ is total in $\mathscr{F}_s(\mathscr{H})$.

(c) (commutation relations) For each $\psi \in F_0$ and $f, g \in \mathscr{H}$,

$$\Phi_S(f)\Phi_S(g)\psi - \Phi_S(g)\Phi_S(f)\psi = i\,\mathrm{Im}(f,g)_{\mathscr{H}}\psi \tag{X.64}$$

Further, if $W(f)$ denotes the unitary operator $e^{i\Phi_S(f)}$, then

$$W(f+g) = e^{-i\,\mathrm{Im}(f,g)/2}W(f)W(g) \tag{X.65}$$

(d) (continuity) If $f_n \to f$ in $\mathscr{H}$, then

$$W(f_n)\psi \to W(f)\psi \qquad \text{for all } \psi \in \mathscr{F}_s(\mathscr{H})$$
$$\Phi_S(f_n)\psi \to \Phi_S(f)\psi \qquad \text{for all } \psi \in F_0$$

(e) For every unitary operator U on $\mathscr{H}$, $\Gamma(U)$: $D(\overline{\Phi_S(f)}) \to D(\overline{\Phi_S(Uf)})$ and for $\psi \in D(\overline{\Phi_S(Uf)})$,

$$\Gamma(U)\overline{\Phi_S(f)}\Gamma(U)^{-1}\psi = \overline{\Phi_S(Uf)}\psi$$

for all $f \in \mathscr{H}$.

Proof Let $\psi \in \mathscr{H}_s^{(n)}$. Since $\Phi_S(f)$: $F_0 \to F_0$, ψ is in $C^\infty(\Phi_S(f))$. Further, it follows from (X.62), (X.63), and the fact that $\|b^-(f)\| = \|f\|$, that

$$\|\underbrace{a^\#(f)\cdots a^\#(f)}_{k \text{ times}}\psi\| \le \sqrt{n+1}\cdots\sqrt{n+k}\,\|f\|^k\|\psi\|$$

where $a^\#(f)$ represents either $a^-(f)$ or $(a^-(f))^*$. Therefore,

$$\|(\Phi_S(f))^k\psi\| \le 2^{k/2}((n+k)!)^{1/2}\|f\|^k\|\psi\|$$

Since $\sum_{k=0}^\infty t^k 2^{k/2}((n+k)!)^{1/2}\|f\|^k/k! < \infty$ for all t, ψ is an analytic vector for $\Phi_S(f)$. Since F_0 is dense in $\mathscr{F}_s(\mathscr{H})$ and is left invariant by Φ_S, $\Phi_S(f)$ is essentially self-adjoint on F_0 by Nelson's analytic vector theorem (Theorem X.39).

The proof of (b) is left as Problem 43.

To prove (c) one first computes that if $\psi \in F_0$, then

$$a^-(f)a^-(g)^*\psi - a^-(g)^*a^-(f)\psi = (f,g)\psi \tag{X.66}$$

(X.64) follows immediately. Although (X.64) and (X.65) are formally equivalent, (X.64) by itself does not imply (X.65) (for an example of how misleading such formal calculations can be, see Section VIII.5). We sketch a proof of (X.65) which uses special properties of the vectors in F_0.

Let $\psi \in \mathscr{H}_s^{(p)}$. Then

$$\|\Phi_S(f)^n \Phi_S(g)^m \psi\| \leq 2^{(n+m)/2} \sqrt{p+1} \cdots \sqrt{p+n+m}\, \|f\|^n \|g\|^m \|\psi\|$$

which implies that $\sum_{n,m} (\|\Phi_S(f)^n \Phi_S(g)^m \psi\|/n!\, m!) t^n t^m$ converges for all t. Since ψ is an analytic vector for $\Phi_S(g)$, $\sum_m ((i\Phi_S(g))^m/m!)\psi = e^{i\Phi_S(g)}\psi$. Further, for each n, $e^{i\Phi_S(g)}\psi$ is in the domain of $\overline{(\Phi_S(f))}^n$ since

$$\sum_{m=0}^{M} \frac{(i\Phi_S(g))^m}{m!}\psi$$

is in it and $\Phi_S(f)^n \sum_{m=0}^{M} ((i\Phi_S(g))^m/m!)\psi$ converges as $M \to \infty$. Thus the estimate

$$\sum_{n,m} \frac{\|(\Phi_S(f))^n (\Phi_S(g))^m\|}{n!\, m!} t^n t^m < \infty$$

shows that $e^{i\Phi_S(g)}\psi$ is an analytic vector for $\Phi_S(f)$ and therefore $e^{i\Phi_S(f)}$ can be computed by the power series. Thus

$$e^{i\Phi_S(f)} e^{i\Phi_S(g)}\psi = \sum_{n,m} \frac{(i\Phi_S(f))^n (i\Phi_S(g))^m}{n!\, m!}\psi$$

Similarly,

$$e^{-it^2 \operatorname{Im}(f,g)/2} e^{it\Phi_S(f+g)}\psi = \sum_{n,m=0}^{\infty} \frac{1}{m!}\frac{1}{n!}\left[\left(-\frac{it^2}{2}\operatorname{Im}(f,g)\right)^m (it\Phi_S(f+g))^n\right]\psi$$

converges absolutely. Direct computations using (X.64) now show that (X.65) holds by a term-by-term comparison of the convergent power series.

To prove (d) let $\psi \in \mathscr{H}_s^{(k)}$ and suppose that $f_n \xrightarrow{\mathscr{K}} f$. Then

$$\|\Phi_S(f_n)\psi - \Phi_S(f)\psi\| \leq \sqrt{2}\sqrt{k+1}\, \|f_n - f\|\, \|\psi\|$$

so $\Phi_S(f_n)\psi \to \Phi_S(f)\psi$. Thus, $\Phi_S(f_n)$ converges strongly to $\Phi_S(f)$ on F_0. Since F_0 is a core for all $\Phi_S(f_n)$ and $\Phi_S(f)$, Theorems VIII.21 and VIII.25 imply that $e^{it\Phi_S(f_n)}\psi \to e^{it\Phi_S(f)}\psi$ for all $\psi \in \mathscr{F}_s(\mathscr{H})$.

To prove (e), let $\eta \in \mathscr{H}^{(n)}$ be of the form $\eta = \psi_1 \otimes \cdots \otimes \psi_n$. Then

$$\begin{aligned}
\Gamma(U) b^-(f) \Gamma(U)^{-1} \eta &= \Gamma(U) b^-(f)(U^{-1}\psi_2 \otimes \cdots \otimes U^{-1}\psi_n) \\
&= \Gamma(U)(f, U^{-1}\psi_1)(U^{-1}\psi_2 \otimes \cdots \otimes U^{-1}\psi_n) \\
&= (Uf, \psi_1)(\psi_2 \otimes \cdots \otimes \psi_n) \\
&= b^-(Uf)\eta
\end{aligned}$$

Since finite linear combinations of such η are dense in $\mathscr{H}^{(n)}$ and $b^-(g)$ has norm $\|g\|$, we conclude that $\Gamma(U)b^-(f)\Gamma(U)^{-1} = b^-(Uf)$. But N and S commute with $\Gamma(U)$, so this immediately implies that $\Gamma(U)a^-(f)\Gamma(U)^{-1} = a^-(Uf)$ on F_0. Taking adjoints and restricting to F_0 we also have $\Gamma(U)(a^-(f))^*\Gamma(U)^{-1} = (a^-(Uf))^*$. Thus, for $\psi \in F_0$, $\Gamma(U)\Phi_S(f)\Gamma(U)^{-1}\psi = \Phi_S(Uf)\psi$. Since the operators on both the right- and left-hand sides of this equality are essentially self-adjoint on F_0, we conclude that

$$\Gamma(U)\overline{\Phi_S(f)}\Gamma(U)^{-1} = \overline{\Phi_S(Uf)} \quad \blacksquare$$

Henceforth we use $\Phi_S(f)$ to denote the closure of $\Phi_S(f)$.

We can now use the Segal quantization to define the free Hermitian scalar field of mass m. We take $\mathscr{H} = L^2(H_m, d\Omega_m)$, where H_m, $m \geq 0$, is the mass hyperboloid in $\mathbb{R}^4$ consisting of those $p \in \mathbb{R}^4$ satisfying $p \cdot \tilde{p} - m^2 = 0$ and $p_0 > 0$, and Ω_m is the Lorentz invariant measure (defined in Section IX.8). For each $f \in \mathscr{S}(\mathbb{R}^4)$ we define Ef in $\mathscr{H}$ by $Ef = \sqrt{2\pi}\hat{f} \restriction H_m$ where (for this section only) the Fourier transform

$$\hat{f}(p) = \frac{1}{(2\pi)^2}\int e^{ip\cdot\tilde{x}} f(x)\, dx$$

is defined in terms of the Lorentz invariant inner product $p \cdot \tilde{x}$. The reason for the extra $\sqrt{2\pi}$ in our definition of E and the plus sign in the definition of Fourier transform is that if f is the distribution $f(\mathbf{x}) = g(\mathbf{x})\delta(t)$, then $\sqrt{2\pi}\,\hat{f}$ is the ordinary three-dimensional Fourier transform of g. If $\Phi_S(\cdot)$ is the Segal quantization over $L^2(H_m, d\Omega_m)$, we define for each *real-valued* $f \in \mathscr{S}(\mathbb{R}^4)$

$$\Phi_m(f) = \Phi_S(Ef) \tag{X.67a}$$

For arbitrary $f \in \mathscr{S}(\mathbb{R}^4)$, we define

$$\Phi_m(f) = \Phi_m(\operatorname{Re} f) + i\Phi_m(\operatorname{Im} f) \tag{X.67b}$$

The mapping $f \mapsto \Phi_m(f)$ is called the **free Hermitian scalar field of mass** m.

On $L^2(H_m, d\Omega_m)$ we define the following unitary representation of the restricted Poincaré group:

$$(U_m(a, \Lambda)\psi)(p) = e^{ip\cdot\tilde{a}}\psi(\Lambda^{-1}p) \tag{X.68}$$

where we are using Λ to denote both an element of the abstract restricted Lorentz group and the corresponding element in the standard representation on $\mathbb{R}^4$. As before F_0 will denote the finite particle vectors.

Theorem X.42 The quadruple

$$\langle \mathscr{F}_s(L^2(H_m, d\Omega_m)), \Gamma(U_m(\cdot, \cdot)), \Phi_m(\cdot), F_0 \rangle$$

satisfies the Wightman axioms. Further, for each $f \in \mathscr{S}(\mathbb{R}^4)$,

$$\Phi_m((\Box^2 + m^2)f) = 0$$

where $\Box^2 = \partial^2/\partial t^2 - \Delta$.

Proof Since $\Omega_m(\cdot)$ is invariant under $\mathscr{L}_+^\uparrow$, $U_m(\cdot, \cdot)$ is a continuous unitary representation of $\mathscr{P}_+^\uparrow$ on $L^2(H_m, d\Omega_m)$. By definition, $\Gamma(U)$ is the strongly continuous unitary group $\bigotimes_{k=1}^n U_m(\cdot, \cdot)$ on $\mathscr{H}_s^{(n)}$ for each n. Thus $\Gamma(U_m)$ is a unitary group on $\mathscr{F}_s(L^2(H_m, d\Omega_m))$ and since $\Gamma(U)$ is strongly continuous on F_0, it is strongly continuous on $\mathscr{F}_s$. This verifies that Property 1 holds.

To verify Property 2, we must show that the four-parameter unitary group $\Gamma(U_m(a, I))$ has spectrum with support in the forward light cone. First notice that $L^2(H_m, d\Omega_m)$ is already a spectral representation for $U_m(a, I)$ since $(\eta, U_m(a, I)\eta) = \int_{H_m} e^{ip \cdot \tilde{a}} |\eta(p)|^2 \, d\Omega_m(p)$. Since $\Gamma(U_m(a, I)) \upharpoonright \mathscr{H}_s^{(n)} = \bigotimes_{k=1}^n U_m(a, I)$, if $\eta \in \mathscr{H}_s^{(n)}$, and $n > 0$, then

$$(\eta, \Gamma(U_m(a, I))\eta) = \int_{\mathbb{R}^4} \cdots \int_{\mathbb{R}^4} \exp\left(i\left(\sum_{i=1}^n p_i\right) \cdot \tilde{a}\right) |\eta(p_1, \ldots, p_n)|^2 \prod_{i=1}^n d\Omega_m(p_i)$$

$$= \int_{\mathbb{R}^4} e^{i\lambda \cdot \tilde{a}} \, d\mu_\eta(\lambda)$$

where $\mu_\eta(S) = \int \cdots \int_{\sum p_i \in S} |\eta(p_1, \ldots, p_n)|^2 \prod_{i=1}^n d\Omega_m(p_i)$. Since Ω_m has support in $\overline{V}_+$ and $\overline{V}_+$ is a cone, μ_η also has support in $\overline{V}_+$. Now, if $\psi = \{\psi^{(n)}\}_{n=0}^\infty$ is a general vector in $\mathscr{F}_s(L^2(H_m, d\Omega_m))$ and μ_ψ the spectral measure so that

$$(\psi, \Gamma(U_m(a, I))\psi) = \int e^{ip \cdot \tilde{a}} \, d\mu_\psi(p)$$

then $\mu_\psi = \sum_{n=0}^\infty \mu_{\psi^{(n)}}$, since $\Gamma(U_m)\colon \mathscr{H}_s^{(n)} \to \mathscr{H}_s^{(n)}$.

The vector $\Omega_0 = \{1, 0, 0, \ldots\}$ is invariant under $\Gamma(U_m(\cdot, \cdot))$ since by definition $\Gamma(U_m)$ acts like the identity on $H_s^{(0)} = \mathbb{C}$. Since no nonzero vector in $L^2(H_m, d\Omega_m)$ is invariant under $U_m(a, I)$ for all $a \in \mathbb{R}^4$, there is no nonzero vector in $\mathscr{H}_s^{(n)}$ which is invariant under $\bigotimes_{k=1}^n U_m(\cdot, I)$. Since $\Gamma(U_m)\colon \mathscr{H}_s^{(n)} \to \mathscr{H}_s^{(n)}$, this implies that the only nonzero invariant vector in $\mathscr{F}_s(L^2(H_m, d\Omega_m))$ is (all scalar multiples of) Ω_0. This verifies Property 3.

Property 4 follows immediately from the definition of Φ_m: $\Phi_m(f) = \Phi_S(Ef)$ for real f and $\Phi_m(f) = \Phi_m(\mathrm{Re}\, f) + i\Phi_m(\mathrm{Im}\, f)$ for complex-valued f, and the fact that $\Phi_S(f)$: $F_0 \to F_0$.

Suppose that $\psi_1, \psi_2 \in F_0$ and $f_n \to f \in \mathscr{S}(\mathbb{R}^n)$ with f_n real-valued. Then

$$Ef_n = \sqrt{2\pi}\, \hat{f}_n \restriction H_m \xrightarrow{L^2(H_m,\, d\Omega_m)} \sqrt{2\pi}\, \hat{f} \restriction H_m = Ef$$

Thus from Theorem X.41d we conclude that

$$(\psi_1, \Phi_m(f_n)\psi_2) \to (\psi_1, \Phi_m(f)\psi_2)$$

By treating the real and imaginary parts of f separately we therefore obtain $(\psi_1, \Phi_m(\cdot)\psi_2) \in \mathscr{S}'(\mathbb{R}^n)$ verifying Property 5.

To prove the Poincaré invariance of the field, notice that $\Gamma(U_m)$: $F_0 \to F_0$ and that if $\psi \in F_0$ and f is a real-valued function in $\mathscr{S}(\mathbb{R}^4)$, then

$$\begin{aligned}\Gamma(U_m(a, \Lambda))\Phi_m(f)\Gamma(U_m(a, \Lambda))^{-1}\psi &= \Gamma(U_m)\Phi_S(Ef)\Gamma(U_m)^{-1}\psi \\ &= \Phi_S(U_m Ef)\psi\end{aligned}$$

by Theorem X.41e. A change of variables shows that $U_m(a, \Lambda)Ef = E(\langle a, \Lambda\rangle f)$, so $\Gamma(U_m(a, \Lambda))\Phi_m(f)\Gamma(U_m(a, \Lambda))^{-1} = \Phi_m(\langle a, \Lambda\rangle f)$. Since both sides of this expression are linear in f and $\Gamma(U_m)$ is a linear operator, the formula is valid for complex-valued f also.

To prove microscopic causality, we must show that for all $f, g \in \mathscr{S}(\mathbb{R}^4)$ with spacelike separated supports and all $\psi \in F_0$,

$$\Phi_m(f)\Phi_m(g)\psi - \Phi_m(g)\Phi_m(f)\psi = 0 \tag{X.69}$$

Since $\Phi_m(\cdot)$ is linear, it is sufficient to prove (X.69) in the case where f and g are real-valued. Then, by (X.64)

$$\begin{aligned}[\Phi_m(f), \Phi_m(g)]\psi &= [\Phi_S(Ef), \Phi_S(Eg)]\psi \\ &= (i\, \mathrm{Im}(Ef, Eg)_{L^2(H_m,\, d\Omega_m)})\psi \\ &= \left(\frac{2\pi}{2}\int_{H_m} (\overline{\hat{f}(p)}\hat{g}(p) - \hat{f}(p)\overline{\hat{g}(p)})\, d\Omega_m(p)\right)\psi \\ &= \left(\int_{\mathbb{R}^4}\int_{\mathbb{R}^4} \frac{1}{2i}\, \Delta_m(x - y) f(x) g(y)\, dx\, dy\right)\psi\end{aligned}$$

where

$$\Delta_m(x) = \frac{i}{2(2\pi)^3}\int (e^{-ip\cdot x} - e^{ip\cdot x})\, d\Omega_m(p)$$

Now, $\Delta_m(x) = \Delta_+(x; m^2) - \Delta_+(-x; m^2)$, so since $\Delta_+(x; m^2) = f_S(x^2)$ for x

spacelike (Theorem IX.48), we conclude that supp $\Delta_m \subset \overline{V}_+ \cup (-\overline{V}_+)$. Thus

$$\iint \Delta_m(x-y)f(x)g(x)\,dx\,dy = 0$$

which implies (X.69).

The cyclicity of the vacuum for $\Phi_m(\cdot)$ follows immediately from Theorem X.41 (parts (b) and (d)) and the fact that the range of the map E on $\mathscr{S}_{\mathbb{R}}(\mathbb{R}^4)$ is dense in $L^2(H_m, d\Omega_m)$ (Problem 44).

Finally, if $f \in \mathscr{S}(\mathbb{R}^4)$, then $\widehat{(\Box^2 + m^2)f}(p) = -(p\cdot\tilde{p} - m^2)\hat{f}(p)$ so

$$E((\Box^2 + m^2)f) = 0$$

Thus $\Phi_m((\Box^2 + m^2)f) = 0$ for all $f \in \mathscr{S}(\mathbb{R}^4)$. ∎

Notice that by the computation above the spectral weight ρ of the Källen–Lehman representation for Φ_m is the point mass at m.

Classical mechanics has provided such a successful framework in physics that it is natural to rephrase physical systems in terms of certain "fixed-time degrees of freedom" which evolve in time. We do this now for the free field by introducing the time-zero field and the canonical conjugate momentum. We emphasize that this choice of a fixed time is not relativistically invariant. As a result, in constructing an interacting field theory by perturbing the free theory using the time-zero fields, it is difficult to recover Lorentz invariance. There is no direct connection between the canonically conjugate momentum and the physical momentum operator P.

We begin in the abstract setting. Recall that a **conjugation** on a Hilbert space $\mathscr{H}$ is an antilinear isometry C so that $C^2 = I$.

Definition Let $\mathscr{H}$ be a complex Hilbert space, $\Phi_S(\cdot)$ the associated Segal quantization. Let C be a conjugation on $\mathscr{H}$ and define $\mathscr{H}_C = \{f \in \mathscr{H} \mid Cf = f\}$. For each $f \in \mathscr{H}_C$ we define $\varphi(f) = \Phi_S(f)$ and $\pi(f) = \Phi_S(if)$. The map $f \mapsto \varphi(f)$ is called the **canonical free field** over $\langle \mathscr{H}, C\rangle$ and the map $f \mapsto \pi(f)$ is called the **canonical conjugate momentum**. We often drop the $\langle \mathscr{H}, C\rangle$ and just write $\mathscr{H}$ if the intended conjugation is clear. Notice that the set of elements of $\mathscr{H}$ for which the maps $f \mapsto \varphi(f)$ and $f \mapsto \pi(f)$ are defined depends on the conjugation C.

Theorem X.43 Let $\mathscr{H}$ be a complex Hilbert space with conjugation C. Let $\varphi(\cdot)$ and $\pi(\cdot)$ be the corresponding canonical fields. Then:

(a) (i) For each $f \in \mathscr{H}_C$, $\varphi(f)$ is essentially self-adjoint on F_0.
(ii) $\{\varphi(f) \mid f \in \mathscr{H}_C\}$ is a commuting family of self-adjoint operators.

(iii) Ω_0 is a cyclic vector for the family $\{\varphi(f) \mid f \in \mathscr{H}_C\}$.

(iv) If $f_n \xrightarrow{\mathscr{H}_C} f$, then

$$\varphi(f_n)\psi \to \varphi(f)\psi \qquad \text{for all } \psi \in F_0$$

and

$$e^{i\varphi(f_n)}\psi \to e^{i\varphi(f)}\psi \qquad \text{for all } \psi \in \mathscr{F}_s(\mathscr{H})$$

(b) Properties (i)–(iv) hold with $\varphi(\cdot)$ replaced by $\pi(\cdot)$.

(c) If $f, g \in \mathscr{H}_C$, then

$$\varphi(f)\pi(g)\psi - \pi(g)\varphi(f)\psi = i(f, g)\psi \qquad \text{for all } \psi \in F_0 \tag{X.70}$$

$$e^{i\varphi(f)}e^{i\pi(g)} = e^{-i(f, g)}e^{i\pi(g)}e^{i\varphi(f)} \tag{X.71}$$

Proof Parts (a)(i) and (a)(iv) follow immediately from the corresponding properties of $\Phi_S(\cdot)$ proven in Theorem X.41. Part (a)(iii) is left to the reader (Problem 43). To see that $\{\varphi(f) \mid f \in \mathscr{H}_C\}$ is a commuting family, notice that (X.65) implies

$$e^{it\varphi(f)}e^{is\varphi(g)} = e^{-its\,\mathrm{Im}(f, g)}e^{is\varphi(g)}e^{it\varphi(f)}$$

where we have used the fact that $\varphi(\cdot)$ is real linear. If $f, g \in \mathscr{H}_C$, then it follows from polarization that $(f, g) = (Cf, Cg) = (g, f)$, so $\mathrm{Im}(f, g) = 0$. Thus $e^{it\varphi(f)}e^{is\varphi(g)} = e^{is\varphi(g)}e^{it\varphi(f)}$ for all s and t. Therefore, by Theorem VIII.13, $\varphi(f)$ and $\varphi(g)$ commute.

The proof of (b) is similar to the proof of (a). (X.70) and (X.71) follow immediately from (X.64), (X.65), and the fact that if $f, g \in \mathscr{H}_C$, then $\mathrm{Im}(f, ig) = \mathrm{Re}(f, g) = (f, g)$. ∎

We now define the conjugation which we will use for the free scalar field of mass m. We write $f \in L^2(H_m, d\Omega_m)$ as $f(p_0, \mathbf{p})$ and define $(Cf)(p_0, \mathbf{p}) = \overline{f(p_0, -\mathbf{p})}$. Notice that C is well-defined on $L^2(H_m, d\Omega_m)$ since $\langle p_0, \mathbf{p}\rangle \in H_m$ if and only if $\langle p_0, -\mathbf{p}\rangle \in H_m$. C is clearly a conjugation. We denote the canonical fields corresponding to C by $\varphi(\cdot)$ and $\pi(\cdot)$ and define

$$\varphi_m(f) = \varphi(Ef)$$
$$\pi_m(f) = \pi(\mu Ef), \qquad \mu = \sqrt{\mathbf{p}^2 + m^2}$$

for real-valued $f \in \mathscr{S}(\mathbb{R}^4)$, extending to all of $\mathscr{S}(\mathbb{R}^4)$ by linearity. In terms of a^-,

$$\varphi_m(f) = \frac{1}{\sqrt{2}}\{(a^-(Ef))^* + a^-(CEf)\}$$

$$\pi_m(f) = \frac{i}{\sqrt{2}}\{(a^-(\mu Ef))^* - a^-(C\mu Ef)\}$$

We warn the reader that the a's in these last formulas differ from those most often used in discussing the free field and that the correct space–time free field is Φ_m and not φ_m; as we will discuss below, φ_m and π_m are useful for discussing the time-zero field. The maps $f \mapsto \varphi_m(f)$ and $f \mapsto \pi_m(f)$ are complex linear and $\varphi_m(f)$, $\pi_m(f)$ are self-adjoint if and only if $Ef \in \mathscr{H}_C$.

Because of the projection E we can extend the class of functions on which $\varphi_m(\cdot)$ and $\pi_m(\cdot)$ are defined to include distributions of the form $\delta(t - t_0)g(x_1, x_2, x_3)$ where $g \in \mathscr{S}(\mathbb{R}^3)$. In particular, if $t_0 = 0$, g is real-valued, and $\hat{g}$ is the *usual* Fourier transform on $\mathbb{R}^3$, then

$$\overline{(CE\widehat{\delta g})(p_0, \mathbf{p})} = \overline{E\widehat{\delta g}(p_0, -\mathbf{p})} = (2\pi)^{-1/2}\overline{\hat{g}(-\mathbf{p})} = (2\pi)^{-1/2}\hat{g}(\mathbf{p}) = E\widehat{\delta g}$$

Thus $E(\delta g)$ and $\mu E(\delta g)$ are in $\mathscr{H}_C$. Therefore $\varphi_m(\delta g)$ and $\pi_m(\delta g)$ are self-adjoint if $g \in \mathscr{S}(\mathbb{R}^3)$ is real. For obvious reasons, the maps $g \mapsto \varphi_m(\delta g)$, $g \mapsto \pi_m(\delta g)$ are called the **time-zero fields**. From now on we will only use test functions of the form δg in $\varphi_m(\cdot)$ and $\pi_m(\cdot)$ and write $\varphi_m(g)$ and $\pi_m(g)$ if $g \in \mathscr{S}(\mathbb{R}^3)$ instead of $\varphi_m(\delta g)$ and $\pi_m(\delta g)$. If f and g are real-valued functions in $\mathscr{S}(\mathbb{R}^3)$, then (X.70) implies that for $\psi \in F_0$,

$$[\varphi_m(f), \pi_m(g)]\psi = i\int_{H_m} \overline{\hat{f}(p)}\hat{g}(p)\mu(p)\psi \, d\Omega_m(p) \tag{X.72}$$

For convenience and also so that our notation coincides with the standard terminology, we now transfer the fields we have constructed from the Fock space built up from $L^2(H_m, d\Omega_m)$ to the Fock space built up from $L^2(\mathbb{R}^3)$. For notational simplicity, we define for $f \in L^2(H_m, d\Omega_m)$

$$a^\dagger(f) = (a^-(f))^*, \qquad a(f) = a^-(Cf)$$

First notice that each function $f(p) \in L^2(H_m, d\Omega_m)$ is in a natural way a function $f(\mathbf{p}) = f(\mu(\mathbf{p}), \mathbf{p})$ on $\mathbb{R}^3$. For each $f \in L^2(H_m, d\Omega_m)$, we define $(Jf)(\mathbf{p}) = f(\mu(\mathbf{p}), \mathbf{p})/\sqrt{\mu(\mathbf{p})}$. J is a unitary map of $L^2(H_m, d\Omega_m)$ onto $L^2(\mathbb{R}^3)$, so $\Gamma(J)$ is a unitary map of $\mathscr{F}_s(L^2(H_m, d\Omega_m))$ onto $\mathscr{F}_s(L^2(\mathbb{R}^3))$. The annihilation and creation operators on $\mathscr{F}_s(L^2(\mathbb{R}^3))$, $\tilde{a}(\cdot)$, $\tilde{a}^\dagger(\cdot)$, are related to $a(\cdot)$ and $a^\dagger(\cdot)$ by the formulas

$$\tilde{a}\left(\frac{f(\mathbf{p})}{\sqrt{\mu(\mathbf{p})}}\right) = \Gamma(J)a(f)\Gamma(J)^{-1}$$

$$\tilde{a}^\dagger\left(\frac{f(\mathbf{p})}{\sqrt{\mu(\mathbf{p})}}\right) = \Gamma(J)a^\dagger(f)\Gamma(J)^{-1}$$

We use the unitary map $\Gamma(J)$ to carry the Wightman fields over to $\mathscr{F}_s(L^2(\mathbb{R}^3))$ by defining

$$\tilde{\Phi}_m(f) \equiv \Gamma(J)\Phi_m(f)\Gamma(J)^{-1}$$
$$= \frac{1}{\sqrt{2}}\left\{\tilde{a}\left(\tilde{C}\frac{Ef}{\sqrt{\mu}}\right) + \tilde{a}^\dagger\left(\frac{Ef}{\sqrt{\mu}}\right)\right\} \qquad \text{for real-valued } f \in \mathscr{S}(\mathbb{R}^4)$$

$$\tilde{\varphi}_m(f) \equiv \Gamma(J)\varphi_m(f)\Gamma(J)^{-1}$$
$$= \frac{1}{\sqrt{2}}\left\{\tilde{a}\left(\frac{E(f\delta)}{\sqrt{\mu}}\right) + \tilde{a}^\dagger\left(\frac{E(f\delta)}{\sqrt{\mu}}\right)\right\} \qquad \text{for real-valued } f \in \mathscr{S}(\mathbb{R}^3)$$

where $\tilde{C} = JCJ^{-1}$ acts by $(\tilde{C}g)(\mathbf{p}) = \overline{g(-\mathbf{p})}$. *Having established this correspondence, we now drop the* $\sim$ *and the bold face letters;* from now on we will only deal with the fields on $\mathscr{F}_s(L^2(\mathbb{R}^3))$ and three-dimensional momenta. Further, we recall that the restriction of the four-dimensional Fourier transform that we have been using in this section to functions of the form $\delta(x_0)g(x_1, x_2, x_3)$ is the usual three-dimensional Fourier transform. Notice that

$$\check{f} = (\overline{C\hat{f}})$$

so $C\hat{f} = \hat{f}$ if and only if f is real-valued.

For f and g real-valued, (X.72) becomes

$$[\varphi_m(f), \pi_m(g)] = i\int f(x)g(x)\,d^3x \tag{X.73}$$

(X.73) is the Schwartz space form of the canonical commutation relations (CCR). In the Appendix to this section we prove that for each $m > 0$, this representation of the CCR is irreducible and for different m, the representations are inequivalent. Thus, the time-zero fields in the free scalar field theories give rise to different representation of the CCR.

As a final topic before turning to interacting fields we will show how the structures which we have developed are related to the "fields" and "annihilation and creation operators" introduced in physics texts. First we let

$$D_{\mathscr{S}} = \{\psi \mid \psi \in F_0, \psi^{(n)} \in \mathscr{S}(\mathbb{R}^{3n}) \text{ for all } n\}$$

and for each $p \in \mathbb{R}^3$ we define an operator $a(p)$ on $\mathscr{F}_s(L^2(\mathbb{R}^3))$ with domain $D_{\mathscr{S}}$ by

$$(a(p)\psi)^{(n)}(k_1, \ldots, k_n) = \sqrt{n+1}\,\psi^{(n+1)}(p, k_1, \ldots, k_n) \tag{X.74}$$

The adjoint of the operator $a(p)$ is *not* a densely defined operator since it is given formally by

$$(a^\dagger(p)\psi)^{(n)}(k_1, \ldots, k_n) = \frac{1}{\sqrt{n}} \sum_{\ell=1}^{n} \delta(p - k_\ell)\psi^{(n-1)}(k_1, \ldots, k_{\ell-1}, k_{\ell+1}, \ldots, k_n) \tag{X.75}$$

However, $a^\dagger(p)$ is a well-defined quadratic form on $D_{\mathscr{F}} \times D_{\mathscr{F}}$. For example, if $\psi_1 = \{0, \psi^{(1)}, 0, \ldots\}$ and $\psi_2 = \{0, 0, \psi^{(2)}, 0, \ldots\}$, then

$$(\psi_2, a^\dagger(p)\psi_1) = \frac{1}{\sqrt{2}} \int (\overline{\psi^{(2)}(k_1, p)}\psi^{(1)}(k_1) + \overline{\psi^{(2)}(p, k_1)}\psi^{(1)}(k_1))\, dk_1$$

The reader can easily check that the formulas

$$a(g) = \int_{\mathbb{R}^3} a(p)g(-p)\, dp \tag{X.76a}$$

$$a^\dagger(g) = \int_{\mathbb{R}^3} a^\dagger(p)g(p)\, dp \tag{X.76b}$$

hold for all $g \in \mathscr{S}(\mathbb{R}^3)$ if the equalities are understood in the sense of quadratic forms. That is, (X.76a) means that for $\psi_1, \psi_2 \in D_{\mathscr{F}}$, we have

$$(\psi_1, a(g)\psi_2) = \int_{\mathbb{R}^3} (\psi_1, a(p)\psi_2)g(-p)\, dp$$

and similarly for (X.76b). Since $a(p)$: $D_{\mathscr{F}} \to D_{\mathscr{F}}$ the powers of $a(p)$ are well-defined operators on $D_{\mathscr{F}}$. As before we can write down a formal expression for $(a^\dagger(p))^n$, but it does not make sense as an operator, only as a quadratic form on $D_{\mathscr{F}} \times D_{\mathscr{F}}$. Notice that

$$(\psi_1, (a^\dagger(p))^n\psi_2) = ((a(p))^n\psi_1, \psi_2) \tag{X.77}$$

so for each n, $(a^\dagger(p))^n$ and $a(p)^n$ are "adjoints" in the sense of quadratic forms. We could of course have defined the quadratic form $a^\dagger(p)^n$ by (X.77) and then calculated that it arises by taking the nth power of the formal object given by (X.75). Since $a(p_1)$: $D_{\mathscr{F}} \to D_{\mathscr{F}}$, $(\psi_1, a^\dagger(p_2)a(p_1)\psi_2)$ is a well-defined quadratic form for all $\langle p_1, p_2\rangle \in \mathbb{R}^3 \times \mathbb{R}^3$. Notice, however, that $(\psi_1, a(p_1)a^\dagger(p_2)\psi_2)$ does not make sense since $a^\dagger(p_2)$ is only a quadratic form. In general any product $\prod_{i=1}^{N_1} a(p_i)$ is a well-defined operator from $D_{\mathscr{F}}$ to $D_{\mathscr{F}}$ and $\prod_{i=N_1+1}^{N_2} a^\dagger(p_i)$ is a well-defined quadratic form on $D_{\mathscr{F}} \times D_{\mathscr{F}}$. Thus

$$\left(\psi_1, \left(\prod_{i=N_1+1}^{N_2} a^\dagger(p_i)\right)\left(\prod_{i=1}^{N_1} a(p_i)\right)\psi_2\right)$$

is also well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$. One can check directly that if $f_i \in \mathscr{S}(\mathbb{R}^3)$, then as quadratic forms

$$\left(\prod_{i=N_1+1}^{N_2} a^\dagger(f_i)\right)\left(\prod_{i=1}^{N_1} a(f_i)\right) = \int_{\mathbb{R}^{3N_2}} \left(\prod_{i=N_1+1}^{N_2} a^\dagger(p_i)\right)\left(\prod_{i=1}^{N_1} a(-p_i)\right)\left(\prod_{i=1}^{N_2} f(p_i)\right) dp_1 \cdots dp_{N_2} \quad \text{(X.78)}$$

and

$$N = \int_{\mathbb{R}^3} a^\dagger(p)a(p)\, dp \quad \text{(X.79)}$$

The generator of time translations in the free scalar field theory of mass m is given by

$$H_0 = \int_{\mathbb{R}^3} \mu(p)a^\dagger(p)a(p)\, dp \quad \text{(X.80)}$$

H_0 is called the **free Hamiltonian of mass** m. (X.78), (X.79), and (X.80) involve no formal manipulations, but are mathematical statements about quadratic forms.

Theorem X.44 Let n_1 and n_2 be nonnegative integers and suppose that $W \in L^2(\mathbb{R}^{3(n_1+n_2)})$. Then there is a unique operator T_W on $\mathscr{F}_s(L^2(\mathbb{R}^3))$ so that $D_{\mathscr{S}} \subset D(T_W)$ is a core for T_W and

(a) $$T_W = \int_{\mathbb{R}^{3(n_1+n_2)}} W(k_1, \ldots, k_{n_1}, p_1, \ldots, p_{n_2})\left(\prod_{i=1}^{n_1} a^\dagger(k_i)\right)\left(\prod_{i=1}^{n_2} a(p_i)\right) dk\, dp \quad \text{(X.81)}$$

as quadratic forms on $D_{\mathscr{S}} \times D_{\mathscr{S}}$.

Furthermore,

(b) If m_1 and m_2 are nonnegative integers so that $m_1 + m_2 = n_1 + n_2$, then $(1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}$ is a bounded operator with

$$\|(1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}\| \leq C(m_1, m_2)\|W\|_{L^2}$$

In particular, if $m_1 = n_1$ and $m_2 = n_2$, then

$$\|(1+N)^{-n_1/2}T_W(1+N)^{-n_2/2}\| \leq \|W\|_{L^2}$$

(c) $$T_W^* = \int_{\mathbb{R}^{3(n_1+n_2)}} \overline{W(k_1, \ldots, k_{n_1}, p_1, \ldots, p_{n_2})}\left(\prod_{i=1}^{n_2} a^\dagger(p_i)\right)\left(\prod_{i=1}^{n_1} a(k_i)\right) dk\, dp$$

as quadratic forms on $D_{\mathscr{S}} \times D_{\mathscr{S}}$.

(d) If $W_n \to W$ in $L^2(\mathbb{R}^{3(n_1+n_2)})$, then $T_{W_n} \to T_W$ strongly on $D_{\mathscr{S}}$.

(e) F_0 is contained in $D(T_W)$ and $D(T_W^*)$, and on vectors in F_0, T_W and T_W^* are given by the explicit formulas

$$(T_W\psi)^{(\ell-n_2+n_1)} = K(\ell, n_1, n_2)S \times \left[\int W(k_1, \ldots, k_{n_1}, p_1, \ldots, p_{n_2})\psi^{(\ell)}(p_1, \ldots, p_{n_2}, k_{n_1+1}, \ldots, k_{n_1+\ell-n_2})\, dp\right] \tag{X.82a}$$

$$(T_W\psi)^{(n)} = 0 \qquad \text{if } n < n_1 - n_2$$

$$(T_W^*\psi)^{(\ell-n_1+n_2)} = K(\ell, n_2, n_1)S \times \left[\int \overline{W(k_1, \ldots, k_{n_1}, p_1, \ldots, p_{n_2})}\psi^{\ell}(k_1, \ldots, k_{n_1}, p_{n_2+1}, \ldots, p_{n_2+\ell-n_1})\, dk\right] \tag{X.82b}$$

$$(T_W^*\psi)^{(n)} = 0 \qquad \text{if } n < n_2 - n_1$$

where S is the symmetrization operator and

$$K(\ell, n_1, n_2) = \left[\frac{\ell!(\ell + n_1 - n_2)!}{((\ell - n_2)!)^2}\right]^{1/2}$$

Proof For vectors in $D_{\mathscr{S}}$, we define $T_W\psi$ by the formula (X.82a). By the Schwarz inequality and the fact that S is a projection,

$$\|(T_W\psi)^{(\ell-n_2+n_1)}\|^2 \leq K(\ell, n_1, n_2)^2\|W\|^2\,\|\psi^{(\ell)}\|^2$$

If we now define an operator T_W^* on $D_{\mathscr{S}}$ by using the formula in (X.82b), then for all φ and ψ in $D_{\mathscr{S}}$ one easily verifies that

$$(\varphi, T_W\psi) = (T_W^*\varphi, \psi)$$

Thus, T_W is closable and T_W^* is the restriction of the adjoint of T_W to $D_{\mathscr{S}}$. From now on we will use T_W to denote $\overline{T}_W$ and T_W^* to denote the adjoint of T_W. By the definition of T_W, $D_{\mathscr{S}}$ is a core and further, since T_W is bounded on the ℓ-particle vectors in $D_{\mathscr{S}}$, we have $F_0 \subset D(T_W)$. Since the right-hand side of (X.82a) is also bounded on the ℓ-particle vectors, (X.82a) represents T_W on all ℓ-particle vectors. The proof of the statements in (e) about T_W^* are the same.

To prove (b), let $\psi \in D_{\mathscr{S}}$. Then by the above computation

$$\|((1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}\psi)^{(\ell-n_2+n_1)}\|^2 \leq \left(\frac{K(\ell, n_1, n_2)}{(1+\ell-n_2+n_1)^{m_1/2}(1+\ell)^{m_2/2}}\right)^2 \|W\|^2\|\psi^{(\ell)}\|^2$$

so that

$$\begin{aligned}\|(1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}\psi\| &\leq \left(\sup_{\ell<\infty}\frac{K(\ell,n_1,n_2)}{(1+\ell-n_2+n_1)^{m_1/2}(1+\ell)^{m_2/2}}\right)\|W\|\,\|\psi\| \\ &\leq C(m_1,m_2)\|W\|\,\|\psi\|\end{aligned}$$

where

$$C(m_1,m_2)=\sup_{\ell}\frac{K(\ell,n_1,n_2)}{(1+\ell-n_2+n_1)^{m_1/2}(1+\ell)^{m_2/2}}<\infty$$

since $m_1+m_2=n_1+n_2$. In all the sup's only ℓ so that $\ell-n_2+n_1\geq 0$ occur since the other terms are annihilated by the action of T_W. Thus, $(1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}$ extends to a bounded operator on $\mathscr{F}_s(\mathscr{H})$ with norm less than or equal to $C(m_1,m_2)$. If $m_1=n_1$ and $m_2=n_2$, then $C(m_1,m_2)=1$.

To prove (d) we need only note that if $\psi=\{0,\ldots,\psi^{(\ell)},0,\ldots\}\in D_{\mathscr{S}}$ and $W_n\xrightarrow{L^2}W$, then

$$\begin{aligned}\|T_{W_n}\psi-T_W\psi\| &= \|T_{W_n-W}\psi\| \\ &\leq K(\ell,n_1,n_2)\|W_n-W\|\,\|\psi\| \\ &\to 0 \qquad \text{as} \quad n\to\infty\end{aligned}$$

Since $D_{\mathscr{S}}$ consists of finite linear combinations of such vectors, we have shown that T_{W_n} converges strongly on $D_{\mathscr{S}}$ to T_W if $W_n\xrightarrow{L^2}W$.

To prove (a) let $\psi_1,\psi_2\in D_{\mathscr{S}}$ with $\psi_1=\{0,\ldots,\psi_1^{(\ell-n_2+n_1)},0,\ldots\}$ and $\psi_2=\{0,\ldots,\psi_2^{(\ell)},0,\ldots\}$. Then, if $W=(\prod_{i=1}^{n_1}f_i(k_i))(\prod_{i=1}^{n_2}g(p_i))$, the definition of the form $(\prod_{i=1}^{n_1}a^\dagger(k_i))(\prod_{i=1}^{n_2}a(p_i))$ shows that

$$\begin{aligned}(\psi_1,T_W\psi_2)=\int W(k_1,\ldots,k_{n_1},p_1,\ldots,p_{n_2}) \\ \times\left(\psi_1,\left(\prod_{i=1}^{n_1}a^\dagger(k_i)\right)\left(\prod_{i=1}^{n_2}a(p_i)\right)\psi_2\right)dk\,dp \qquad \text{(X.83)}\end{aligned}$$

Since both sides of (X.83) are linear in W, the relationship continues to hold for W's that are finite linear combinations of such products. Since

$$\left(\psi_1,\left(\prod_{i=1}^{n_1}a^\dagger(k_i)\right)\left(\prod_{i=1}^{n_2}a(p_i)\right)\psi_2\right)\in L^2(\mathbb{R}^{3(n_1+n_2)})$$

and since (d) holds, both the right- and left-hand sides of (X.83) are continuous linear functionals on $L^2(\mathbb{R}^{3(n_1+n_2)})$. Since they agree on a dense

set, they agree everywhere. Finally, (X.83) extends by linearity to all of $D_{\mathscr{S}} \times D_{\mathscr{S}}$. This proves (a); the proof of (c) is similar. ∎

Finally, we note that as quadratic forms on $D_{\mathscr{S}}$ we can express the free scalar field and the time zero fields in terms of $a^\dagger(k)$ and $a(k)$:

$$\Phi_m(x, t) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{i(\mu(p)t - p\cdot x)} a^\dagger(p) + e^{-i(\mu(p)t - p\cdot x)} a(p) \frac{d^3p}{\sqrt{2\mu(p)}} \tag{X.84}$$

$$\varphi_m(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} (e^{-ip\cdot x} a^\dagger(p) + e^{ip\cdot x} a(p)) \frac{d^3p}{\sqrt{2\mu(p)}} \tag{X.85}$$

$$\pi_m(x) = \frac{i}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} (e^{-ip\cdot x} a^\dagger(p) - e^{ip\cdot x} a(p)) \sqrt{\frac{\mu(p)}{2}}\, d^3p \tag{X.86}$$

* * *

Before introducing the Hamiltonian approach for constructing a self-interacting scalar boson field in two-dimensional space–time, it is appropriate to make a few general remarks about interacting quantum field theories. At the present time, most of these theories are premathematical in the following sense. Hamiltonians and fields are written down, but no Hilbert space is given on which they are well-defined operators. The matrix elements of the S-operator are then calculated from the fields and Hamiltonian by formal manipulation. These matrix elements are expressed as power series whose coefficients depend on the vacuum expectation values of a related free field theory. Typically, each coefficient of this power series is given by a divergent integral. One formally cancels these infinities by making various input parameters in the theory infinite and then follows a set of prescriptions for extracting the "principal parts" of the resulting difference of divergent integrals; this is called "renormalization." In quantum electrodynamics, these procedures have produced predictions very close to experimental values. However, only slow progress has been made on the mathematical problem of putting these models on a sound foundation. Substantial mathematical results exist in only a few cases and only in space–time dimensions smaller than 4. In only one model (the theory we discuss below is a special case of this model) have all the Wightman axioms been verified (as of 1974). If these cases are a guide, the mathematical resolution of these problems will require advances in diverse areas of functional analysis: self-adjointness questions, perturbation theory, scattering theory, probability theory, spectral analysis, and C^*-algebras.

An "interacting field theory" is a field theory satisfying the Wightman axioms which has a nontrivial scattering theory (see Section XII.15). A

natural way to construct such fields is to try to make a perturbation of one of the free theories which we have constructed. In classical Lagrangian field theory the simplest Hamiltonians are of the form

$$H = H_0 + \int_{\mathbb{R}^3} F(\varphi(x))\, d^3x$$

where F is some function, say a polynomial (see Section X.13). Since we want the Hamiltonian to be bounded below, we expect that the polynomial should be of even order and the coefficient of the highest term positive. The case $F(x) = \alpha x^2$ turns out to have a trivial scattering theory; in fact, the resulting theory is just the free field of mass $m + 2\alpha$. The next simplest case is $F(x) = \lambda x^4$. Thus, we are led to considering the formal Hamiltonian

$$H = H_0 + \lambda \int_{\mathbb{R}^3} (\varphi_m(x))^4\, d^3x, \qquad \lambda > 0 \tag{X.87}$$

where H_0 is the Hamiltonian of the free scalar boson field theory of mass m and $\varphi_m(x)$ is the free field at time zero. One's first naïve hope would be to show that H is self-adjoint and then define the interacting field on Fock space by

$$\Phi(x, t) = e^{iHt}\varphi_m(x)e^{-iHt} \tag{X.88}$$

We will not be able to make sense of (X.87) and (X.88) without serious modifications, but using the commutation relations between φ, π, a, and $a^\dagger$, we can formally compute the differential equation which $\Phi(x, t)$ satisfies (this is just the kind of formal manipulation which we warned the reader against in Section VIII.5):

$$\frac{\partial^2}{\partial t^2}\Phi(x, t) = e^{iHt}(i^2)[H, [H, \varphi_m(x)]]e^{-iHt}$$

$$\begin{aligned}
[H, \varphi_m(x)] &= [H_0, \varphi_m(x)] \\
&= \iint \frac{\mu(k)}{(2\pi)^{3/2}\sqrt{2\mu(\ell)}} \{e^{+ik\cdot x}[a^\dagger(k)a(k), a(\ell)] \\
&\quad + e^{-ik\cdot x}[a^\dagger(k)a(k), a^\dagger(\ell)]\}\, dk\, d\ell \\
&= \iint \frac{\mu(k)}{(2\pi)^{3/2}\sqrt{2\mu(\ell)}} \{e^{+ik\cdot x}(-a(k)\delta(k-\ell)) \\
&\quad + e^{-ik\cdot x}a^\dagger(k)\delta(k-\ell)\}\, dk\, d\ell \\
&= \int \frac{\sqrt{\mu(k)}}{(2\pi)^{3/2}\sqrt{2}}(-e^{+ik\cdot x}a(k) + e^{-ik\cdot x}a^\dagger(k))\, dk = -i\pi_m(x)
\end{aligned}$$

$$[H, [H, \varphi_m(x)]] = [H_0, [H, \varphi_m(x)]] + [H_I, [H, \varphi_m(x)]]$$

$$[H_0, [H, \varphi_m(x)]] = \int \frac{(\mu(k))^2}{\sqrt{2\mu(k)}\,(2\pi)^{3/2}} (e^{+ik\cdot x}a(k) + e^{-ik\cdot x}a^\dagger(k))\,dk$$

$$= (-\Delta + m^2)\varphi_m$$

$$[\varphi_m(y), [H, \varphi_m(x)]] = \int \frac{e^{-ik\cdot(x-y)}}{(2\pi)^{3/2}}\,d^3k = \delta(x-y)$$

$$[H_I, [H, \varphi_m(x)]] = \lambda \int [\varphi_m(y)^4, [H, \varphi_m(x)]]\,dy$$

$$= 4\lambda \int \varphi_m(y)^3 \delta(x-y)\,dy$$

$$= 4\lambda \varphi_m(x)^3$$

Thus,

$$\frac{\partial^2}{\partial t^2}\Phi(x,t) = e^{iHt}(\Delta - m^2)\varphi_m(x)e^{-iHt} - 4\lambda e^{iHt}\varphi_m(x)^3 e^{-iHt}$$

$$= (\Delta - m^2)e^{iHt}\varphi_m(x)e^{-iHt} - 4\lambda(e^{iHt}\varphi_m(x)e^{-iHt})^3$$

$$= (\Delta - m^2)\Phi(x,t) - 4\lambda\Phi(x,t)^3$$

Thus, formally the field $\Phi(x, t)$ satisfies

$$(\Box^2 + m^2)\Phi(x,t) = -4\lambda(\Phi(x,t))^3 \tag{X.89}$$

Another way of looking at our problem is that we are trying to find an operator-valued distribution $\Phi(x, t)$ which satisfies (X.89) and also satisfies the Wightman axioms. Henceforth, we write $\varphi(x)$ instead of $\varphi_m(x)$.

We now return to the consideration of (X.87). Although $\varphi(x)$ is a well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$, it is not an operator, so we must say what we mean by the fourth power $(\varphi(x))^4$. Suppose that we take the expression for $\varphi(x)$ given by (X.85) and formally take the fourth power as if $\varphi(x)$ were an operator. We get a sum of sixteen terms of the form

$$\underset{\mathbf{R}^3 \cdots \mathbf{R}^3}{\int\int\int\int} \exp\left(-i\sum_{i=1}^4 k_j x\right)\left(\prod_{j=1}^4 (2\pi)^{-3/2}(2\mu(k_j))^{-1/2}\right)\left(\prod_{j=1}^4 a^\#(k_j)\right) dk_1 \cdots dk_4 \tag{X.90}$$

where $a^\#(k_j)$ stands for either $a(-k_j)$ or $a^\dagger(k_j)$. As we have already learned, expressions of the form (X.90) do not in general make sense even as quadratic forms unless all the $a^\dagger$ terms are to the left of all the a terms. However,

if all the $a^\dagger$ terms are to the left, then for each x, (X.90) is a well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$. We therefore define the ***n*th Wick power** of $\varphi(x)$ to be the quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$ obtained by formally taking the nth power of $\varphi(x)$ and moving all the $a^\dagger$ terms to the left of the a terms. The nth Wick power of $\varphi(x)$ will be denoted by $:\varphi(x)^n:$. We note that the nth Wick power should really be called the nth Wick power *with respect to* Ω_0 (see Problem 48). The reader can check that *formally*

$$:\varphi(x)^4: = \varphi(x)^4 - c\varphi(x)^2 + d$$

where c and d are appropriately chosen infinite constants. By putting in cut-offs we will later make precise mathematical sense out of this statement.

If we now replace $(\varphi(x))^4$ by $:\varphi(x)^4:$ in (X.87), then H is a well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$. For example, if $\psi_i = \{0, 0, 0, \psi_i^{(3)}, 0, \ldots\}$, $i = 1, 2$, then the term in $(\psi_1, H\psi_2)$ with two $a^\dagger$'s and two a's is

$$\int \left(\iiiint \left(\frac{\exp(-ix(k_1 + k_2 - k_3 - k_4))}{\prod_{j=1}^4 (2\mu(k_j))^{1/2}(2\pi)^{3/2}} \right) \times \left(\iint \overline{\psi_1^{(3)}(p_1, k_1, k_2)} \psi_2^{(3)}(p_2, k_3, k_4)\, dp_1\, dp_2 \right) dk_1 \cdots dk_4 \right) dx \quad \text{(X.91)}$$

This is a well-defined finite integral since $\psi_i^{(3)} \in \mathscr{S}(\mathbb{R}^3)$. Unfortunately, this quadratic form does not arise from an operator. To see this, consider the formal expression for $H\Omega_0$. This is a vector $(0, 0, 0, 0, \psi^{(4)}, 0, \ldots)$ with (formally)

$$\psi^{(4)}(k_1, k_2, k_3, k_4) = \int_{\mathbb{R}^3} \frac{\exp(-ix \sum_{i=1}^4 k_i)}{\prod_{i=1}^4 (2\pi)^{3/2}(2\mu(k_i))^{1/2}}\, dx$$

$$= \frac{\delta(\sum_{i=1}^4 k_i)}{(2\pi)^{9/2} \prod_{i=1}^4 (2\mu(k_i))^{1/2}}$$

This expression is certainly not in $L^2(\mathbb{R}^{(3)(4)})$; first, of course, it is singular because of the delta function, but even if we restrict the x integration by letting $g \in C_0^\infty(\mathbb{R}^3)$ and consider

$$\int \frac{g(x)\exp(-ix \sum_{i=1}^4 k_i)}{\prod_{i=1}^4 (2\pi)^{3/2}(2\mu(k_i))^{1/2}}\, dx = \frac{\hat{g}(\sum_{i=1}^4 k_i)}{(2\pi)^{9/2} \prod_{i=1}^4 (2\mu(k_i))^{1/2}}$$

we still do not get an L^2 function because $\mu(k_i)$ grows too slowly at ∞. Thus, there are two kinds of infinities involved here: the infinite volume (x space) divergence and the ultraviolet (large k) divergence.

In order to obtain an operator, we *restrict ourselves to one space dimension* (i.e., each of the k_i, p_i, and x are now one dimensional) and replace the quadratic form $\int_{\mathbb{R}} :\varphi(x)^4:\, dx$ by $\int_{\mathbb{R}} g(x):\varphi(x)^4:\, dx$ where $g(x)$ is a real-valued

function in $L^2(\mathbb{R})$. Then, each of the terms in the quadratic form

$$H_0 + \int_{\mathbb{R}} g(x):\varphi(x)^4: dx$$

has a kernel of the form $\hat{g}(\sum_{j=1}^4 k_j)/\prod_{j=1}^4 (2\mu(k_j))^{1/2}$. Since this function is in $L^2(\mathbb{R}^4)$ (Problem 47), we are guaranteed by Theorem X.44 that the quadratic form arises from an operator on $D_{\mathscr{S}}$ which is symmetric since g is real-valued. We denote by $H_I(g)$ the operator $\int_{\mathbb{R}} g(x):\varphi(x)^4: dx$ and define on $D_{\mathscr{S}}$

$$H(g) = H_0 + H_I(g) = H_0 + \int_{\mathbb{R}} g(x):\varphi(x)^4: dx$$

We will often choose for g a smooth function of compact support which equals one on a very large interval. Occasionally, one takes the characteristic function of a large interval for g. In either case, the effect of g is to turn off the interaction for large values of x. Therefore, g is called a **space cut-off** and $H(g)$ is called the **spatially cut-off Hamiltonian for the $(\varphi^4)_2$ field theory** (the 2 refers to the fact that we are using only one space dimension, so space–time is two dimensional). We summarize in a proposition.

Proposition Let φ be the free scalar boson field of mass m at $t = 0$ in two-dimensional space–time. Let g be a real-valued function in $L^2(\mathbb{R})$. Then

$$H(g) = H_0 + H_I(g) = \int_{\mathbb{R}} \mu(k)a^\dagger(k)a(k)\, dk + \int_{\mathbb{R}} g(x):\varphi(x)^4: dx$$

is a well-defined symmetric operator on $D_{\mathscr{S}}$.

In Section 9 we will show that $H(g)$ is essentially self-adjoint on $C^\infty(H_0) \cap D(H_I(g))$. In Chapter XIX we will show how von Neumann algebras can be used to remove the spatial cut-off by choosing a new representation of the canonical commutation relations.

The procedure that we have just indicated for controlling the infinite volume infinity by putting in a spatial cut-off which is then removed by C^*-algebra techniques is generally believed to be the correct method for handling this infinity in more general quantum field theories. It is thought that the ultraviolet divergences in $(\varphi^4)_3$ and $(\varphi^4)_4$ can be removed by a procedure known as renormalization together with a change of representation of the commutation relations. To describe renormalization very briefly recall that we have seen that the Wick ordering of powers of the

field can be interpreted as subtracting a lower order polynomial with infinite coefficients. In $(\varphi^4)_3$ it is known, and in $(\varphi^4)_4$ it is expected, that a similar procedure of subtracting terms with infinite constants will work except that the constants will no longer be linear in λ as they are for Wick ordering. For further discussion and references to the $(\varphi^4)_3$ results, see the Notes.

Our final topic is the construction of Q-space and $L^2(Q, d\mu)$, another representation of the Fock space structures which we have presented. In analogy with the one degree of freedom case where $\mathscr{F}(\mathbb{R})$ is isomorphic to $L^2(\mathbb{R}, dx)$ in such a way that $\Phi_S(1)$ becomes multiplication by x, we will construct a measure space $\langle Q, \mu\rangle$, with $\mu(Q) = 1$, and a unitary map S: $\mathscr{F}_s(\mathscr{H}) \to L^2(Q, d\mu)$ so that for each $f \in \mathscr{H}_C$, $S\varphi(f)S^{-1}$ acts on $L^2(Q, d\mu)$ by multiplication by a measurable function. We can then show that in the case of the free scalar field of mass m in two-dimensional space-time, $V \equiv SH_I(g)S^{-1}$ is just multiplication by a function $V(q)$ which is in $L^p(Q, d\mu)$ for each $p < \infty$. In Section X.9, we will use this property of V in a proof that $H = H_0 + H_I(g)$ is essentially self-adjoint on $C^\infty(H_0) \cap D(H_I(g))$.

Let $\{f_n\}_{n=1}^\infty$ be an orthonormal basis for $\mathscr{H}$ so that each $f_n \in \mathscr{H}_C$ and let $\{g_k\}_{k=1}^N$ be a finite collection of the f_n. Let $\mathscr{F}_N$ be the closure of the set

$$\{P(\varphi(g_1), \ldots, \varphi(g_N))\Omega_0 \,|\, P \text{ a polynomial}\}$$

in $\mathscr{F}_s(\mathscr{H})$ and define $F_0^{(N)} = \mathscr{F}_N \cap F_0$. From Theorem X.43 (and its proof) it follows that $\varphi(g_k)$ and $\pi(g_\ell)$ are essentially self-adjoint on $F_0^{(N)}$ and that

$$e^{it\varphi(g_k)}e^{is\pi(g_\ell)} = e^{-ist\delta_{k\ell}}e^{is\pi(g_\ell)}e^{it\varphi(g_k)}$$

Thus we have a representation of the Weyl relations in which the vector Ω_0 satisfies $(\varphi(g_k)^2 + \pi(g_k)^2 - 1)\Omega_0 = 0$ and is cyclic for the operators $\{\varphi(g_k)\}_{k=1}^N$. Therefore by the construction in Problem 30 (or we could appeal directly to Theorem VIII.14), there is a unitary map $\tilde{S}^{(N)}$: $\mathscr{F}_N \to L^2(\mathbb{R}^N)$ so that

$$\tilde{S}^{(N)}\varphi(g_k)(\tilde{S}^{(N)})^{-1} = x_k$$

$$\tilde{S}^{(N)}\pi(g_k)(\tilde{S}^{(N)})^{-1} = \frac{1}{i}\frac{d}{dx}$$

and

$$\tilde{S}^{(N)}\Omega_0 = \pi^{-N/4}\exp\left(-\sum_{k=1}^N \frac{x_k^2}{2}\right)$$

It is convenient to use the Hilbert space $L^2(\mathbb{R}^N, \pi^{-N/2}\exp(-\sum_{k=1}^N x_k^2)\, d^N x)$ instead of $L^2(\mathbb{R}^N)$ so let $d\mu_k = \pi^{-1/2}e^{-x_k^2}\, dx_k$ and define $(Tf)(x) = \pi^{N/4}\exp(\sum_{k=1}^N x_k^2/2)f(x)$. Then T is a unitary map of $L^2(\mathbb{R}^N)$ onto

$L^2(\mathbb{R}^N, \prod_{k=1}^N d\mu_k)$ and if we let $S^{(N)} = T\tilde{S}^{(N)}$, we have

$$S^{(N)}: \mathscr{F}_N \to L^2\left(\mathbb{R}^N, \prod_{k=1}^N d\mu_k\right)$$

$$S^{(N)}\varphi(g_k)(S^{(N)})^{-1} = x_k$$

$$S^{(N)}\pi(g_k)(S^{(N)})^{-1} = -\frac{x_k}{i} + \frac{1}{i}\frac{\partial}{\partial x_k}$$

$$S^{(N)}\Omega_0 = 1 \qquad \text{(the function identically one)}$$

Notice that each μ_k has mass one, which implies that

$$\begin{aligned}(\Omega_0, P_1(\varphi(g_1)) \cdots P_N(\varphi(g_N))\Omega_0) &= \int_{\mathbb{R}^N} P_1(x_1) \cdots P_N(x_N) \prod_{k=1}^N d\mu_k \\ &= \prod_{k=1}^N \int_{\mathbb{R}} P_k(x_k)\, d\mu_k \\ &= \prod_{k=1}^N (\Omega_0, P_k(\varphi(g_k))\Omega_0) \qquad \text{(X.92)}\end{aligned}$$

where $P_1, \ldots, P_N$ are polynomials. This formula can also be proven, of course, by direct computations on $\mathscr{F}_s(\mathscr{H})$.

Now it is easy to see how to construct $\langle Q, d\mu\rangle$. We define $Q = \times_{k=1}^\infty \mathbb{R}$. Take the σ-algebra generated by countable products of measurable sets in $\mathbb{R}$ and set $\mu = \otimes_{k=1}^\infty \mu_k$. We denote the points of Q by $q = \langle q_1, q_2, \ldots\rangle$. Then $\langle Q, \mu\rangle$ is a measure space and the set of functions of the form $P(q_1, \ldots, q_n)$, where P is a polynomial and n is arbitrary, is dense in $L^2(Q, d\mu)$. For a discussion of the measure-theoretic details, see the references in the Notes. Let P be a polynomial in N variables

$$P(x_{k_1}, \ldots, x_{k_N}) = \sum_{\ell_1, \ldots, \ell_M} c_{\ell_1, \ldots, \ell_N} x_{k_1}^{\ell_1}, \ldots, x_{k_N}^{\ell_N}$$

and define

$$S: P(\varphi(f_{k_1}), \ldots, \varphi(f_{k_N}))\Omega_0 \to P(q_{k_1}, \ldots, q_{k_N})$$

Then

$$\begin{aligned}\|P(\varphi(f_{k_1}), \ldots, \varphi(f_{k_N}))\Omega_0\|^2 &= \sum_{\ell, \mathbf{m}} c_\ell \bar{c}_{\mathbf{m}} (\Omega_0, \varphi(f_{k_1})^{\ell_1 + m_1} \cdots \varphi(f_{k_N})^{\ell_N + m_N}\Omega_0) \\ &= \sum_{\ell, \mathbf{m}} c_\ell \bar{c}_{\mathbf{m}} \int_{\mathbb{R}^N} q_{k_1}^{\ell_1 + m_1} \cdots q_{k_N}^{\ell_N + m_N} \prod_{i=1}^N d\mu_{k_i} \\ &= \int_Q |P(q_{k_1}, \ldots, q_{k_N})|^2\, d\mu\end{aligned}$$

by (X.92) and the fact that each μ_k has mass one. Since Ω_0 is cyclic for polynomials in the fields (Theorem X.42), S extends to a unitary map of $\mathscr{F}_s(\mathscr{H})$ onto $L^2(Q, d\mu)$. Clearly $S\varphi(f_k)S^{-1} = q_k$ and $S\Omega_0 = 1$.

Theorem X.45 Let φ_m be the free scalar field of mass m (in two-dimensional space-time) at time zero. Let $g \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ and define

$$H_I(g) = \int_{\mathbb{R}} g(x) :\varphi_m(x)^4: \, dx$$

Let S denote the unitary map of $\mathscr{F}_s(L^2(\mathbb{R}))$ onto $L^2(Q, d\mu)$ constructed above. Then $V \equiv SH_I(g)S^{-1}$ is multiplication by a function $V(q)$ which satisfies:

(a) $V \in L^p(Q, d\mu)$ for all $p < \infty$.
(b) $e^{-tV} \in L^1(Q, d\mu)$ for all $t \in [0, \infty)$.

Proof We will prove (a). See the Notes for a reference for the proof of (b). Let $\chi_n(x)$ be the characteristic function of $(-n, n)$ and define

$$\varphi_m(x, n) = \frac{1}{\sqrt{4\pi}} \int (e^{-ik\cdot x}a(k) + e^{ik\cdot x}a^\dagger(k)) \frac{\chi_n(k)}{\sqrt{\mu(k)}} \, dk$$

Then $\varphi_m(x, n)$ is a well-defined operator-valued *function* of x. We define $:\varphi_m(x, n)^4:$ by moving all the $a^\dagger$'s to the left in the formal expression for $\varphi_m(x, n)^4$. $:\varphi_m(x, n)^4:$ is also a well-defined operator for each x and $:\varphi(x, n)^4:$ takes F_0 into itself. Now define

$$H_I(g, n) = \int_{\mathbb{R}} g(x) :\varphi_m(x, n)^4: \, dx$$

and set $V_n = SH_I(g, n)S^{-1}$. For each x,

$$:\varphi_m(x, n)^4: = \varphi_m(x, n)^4 + d_2(n)\varphi_m(x, n)^2 + d_0(n)$$

where the coefficients d_2 and d_0 are independent of x but dependent on n (Problem 48). For each x, $S\varphi_m(x, n)S^{-1}$ is just the operator on $L^2(Q, d\mu)$ which operates by multiplying by $\sum_{k=1}^{\infty} c_k(x, n)q_k$ where $c_k(x, n) = (2\pi)^{-1/2} \times (f_k, \chi_n\mu^{-1/2}e^{ikx})$. Furthermore, $\sum_{k=1}^{\infty} |c_k(x, n)|^2 = (2\pi)^{-1}\|\chi_n\mu^{-1/2}\|_2^2$, so $S\varphi_m(x, n)^4S^{-1}$ and $S\varphi_m(x, n)^2S^{-1}$ are in $L^2(Q, d\mu)$ and the $L^2(Q, d\mu)$ norms are uniformly bounded in x. Therefore, since $g \in L^1(\mathbb{R})$, $SH_1(g, n)S^{-1}$ operates on $L^2(Q, d\mu)$ by multiplication by an $L^2(Q, d\mu)$ function which we denote by $V_n(q)$.

For each n, $H_I(g, n)$ differs from $H_I(g)$ only in that the kernel in each of the terms is $g(\sum k_i) \prod_{i=1}^4 \mu(k_i)^{-1/2}\chi_n(k_i)$. As $n \to \infty$, these kernels converge to $g(\sum k_i) \prod_{i=1}^4 \mu(k_i)^{-1/2}$ in $L^2(\mathbb{R}^4)$. Therefore, by Theorem X.44, $H_I(g, n)\psi \to$

$H_I(g)\psi$ for $\psi \in F_0$. In particular $H_I(g, n)\Omega_0 \to H_I(g)\Omega_0$. But, since $S\Omega_0 = 1$, $\|H_I(g, n)\Omega_0\| = \|SH_I(g, n)S^{-1}\|_{L^2(Q, d\mu)} = \|V_n\|_{L^2(Q, d\mu)}$. Thus, the sequence of functions V_n is Cauchy in $L^2(Q, d\mu)$ and so converges to a function $V \in L^2(Q, d\mu)$. The reader can now easily complete the proof by showing that each $P(q_1, \ldots, q_n)$ is in the domain of V and $SH_I(g)S^{-1} = V$ on that domain. Since Ω_0 is in the domain of $H_I(g)^n$ for all n, 1 is in the domain of V^n for all n. Thus, for all n, $V \in L^{2n}(Q, d\mu)$. Since $\mu(Q) < \infty$, $V \in L^p(Q, d\mu)$ for all $p < \infty$. ∎

Appendix to X.7 The Weyl relations for the free field

In this appendix, we study the natural generalizations of the Weyl relations (VIII.8) to the case of infinitely many degrees of freedom. Let $\mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$ denote the Schwarz space of real-valued functions on $\mathbb{R}^\nu$. Suppose that $f \mapsto U(f)$ and $f \mapsto V(f)$ are maps of $\mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$ into the bounded operators on a separable Hilbert space $\mathscr{H}$ which satisfy:

(i) for each $f \in \mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$, $V(f)$ and $U(f)$ are unitary;
(ii) for all $f, g \in \mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$, $V(f)$ and $U(f)$ satisfy

$$V(f+g) = V(f)V(g), \qquad U(f+g) = U(f)U(g) \tag{X.93}$$

$$V(f)U(g) = U(g)V(f)\exp\left(-i\int_{\mathbb{R}^\nu} f(x)g(x)\,dx\right) \tag{X.94}$$

(iii) if $f_n \xrightarrow{\mathscr{S}(\mathbb{R}^\nu)} f$, then $U(f_n) \to U(f)$ and $V(f_n) \to V(f)$ strongly on $\mathscr{H}$.

The pair of maps $\{U(\cdot), V(\cdot)\}$ is called a representation of the **Weyl relations** over $\mathscr{S}(\mathbb{R}^\nu)$. Two such representations, $\{U_1(\cdot), V_1(\cdot)\}$ on $\mathscr{H}_1$ and $\{U_2(\cdot), V_2(\cdot)\}$ on $\mathscr{H}_2$, are called **equivalent** if there is a unitary operator $T: \mathscr{H}_1 \to \mathscr{H}_2$, so that $U_2(f) = TU_1(f)T^{-1}$ and $V_2(f) = TV_1(f)T^{-1}$ for all $f \in \mathscr{S}(\mathbb{R}^\nu)$. The relation (X.71) shows that for each m, the pair $\{e^{i\pi_m(\cdot)}, e^{i\varphi_m(\cdot)}\}$, where π_m, φ_m are the time-zero field and conjugate momentum of the free scalar field of mass m, is a representation of the Weyl relations on $\mathscr{F}_s(L^2(\mathbb{R}^3))$. We will see below that these representations are inequivalent.

Let $\{U(\cdot), V(\cdot)\}$ be a representation of the Weyl relations over $\mathscr{S}(\mathbb{R}^\nu)$ and let $\{h_n\}_{n=1}^\infty$ be the orthonormal basis for $L^2(\mathbb{R}^\nu)$ made up of products of Hermite functions. If $U_n(t) = U(th_n)$ and $V_n(t) = V(th_n)$, then (X.93), (X.94), and (iii) imply that for each n, $U_n(t)$ and $V_n(t)$ are strongly continuous unitary groups on $\mathscr{H}$ that satisfy

$$\begin{aligned} V_n(t)U_m(s) &= U_m(s)V_n(t), \qquad m \neq n \\ V_n(t)U_m(s) &= e^{-ist}U_m(s)V_m(t) \end{aligned} \tag{X.95}$$

for all s, $t \in \mathbb{R}$. Thus, for all n, $\{U_n(t), V_n(s)\}$ satisfy the Weyl relations (VIII.8), and for different n the corresponding unitary operators commute. Von Neumann's theorem (Theorem VIII.14, see Problem 30 and Chapter XIV) states that up to multiplicity, there is only one representation (the Schrödinger representation) of the relations (X.95) if n ranges over a finite set of integers. It was thought for a long time that von Neumann's theorem held for the case of infinitely many n, but examples of inequivalent representations occurred in the work of Friedrichs in the late 1940's and were emphasized in the later work of Segal and Gårding–Wightman. As we have already mentioned, Theorem X.46 below shows that the free scalar fields of different masses give rise to inequivalent representations.

By (X.93) and (iii), $V(tf)$ and $U(tf)$ are continuous unitary groups on $\mathscr{H}$; we denote their generators by $\varphi(f)$ and $\pi(f)$ respectively. It can be shown that there is a domain D in $\mathscr{H}$ which is invariant under all of the operators $\varphi(f), \pi(f), f \in \mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$ and on which $\varphi(f)$ and $\pi(f)$ are essentially self-adjoint. For $\psi \in D$, (X.94) implies that

$$[\varphi(f), \pi(g)]\psi = i \int_{\mathbb{R}^\nu} f(x)g(x)\, dx\, \psi \tag{X.96}$$

for all f, $g \in \mathscr{S}(\mathbb{R}^\nu)$. A pair of operator-valued distributions over $\mathscr{S}(\mathbb{R}^\nu)$ which satisfy (X.96) are said to be a representation of the **canonical commutation relations**. In the case of the time-zero free scalar field of mass m, we have already seen that D can be chosen to be D_0 and that (X.96) can be verified directly. As in the case of finitely many p_i and q_i discussed in Section VIII.5, (X.96) does not necessarily imply (X.94) although they are formally equivalent.

We now prove that the representations of the canonical commutation relations arising from free scalar fields of different masses $m > 0$ are inequivalent. A family of bounded operators on a Hilbert space is called **irreducible** if the only operators that commute with all members of the family are scalar multiples of the identity.

Lemma 1 Let $\Phi_S(\cdot)$, be the Segal quantization over a separable Hilbert space $\mathscr{H}$. Then the family of operators $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}$ is irreducible.

Proof Let $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}'$ denote the set of operators which commute with all $e^{i\Phi_S(f)}, f \in \mathscr{H}$. Since $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}'$ is a norm closed algebra of operators closed under taking adjoints, the same proof as in the lemma after Theorem VI.19 shows that each operator in $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}'$ may be written as a linear combination of four unitaries in $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}'$. It is therefore sufficient to prove that every unitary $T \in \{e^{i\Phi(f)} \mid f \in \mathscr{H}\}'$ is a scalar multiple of the identity.

For each $f \in \mathscr{H}$ and all t, T commutes with $e^{it\Phi_S(f)}$ so by Theorem VIII.13, T commutes with the spectral projections of $\Phi_S(f)$. Thus, T: $D(\Phi_S(f)) \to D(\Phi_S(f))$ and $T\Phi_S(f)\psi = \Phi_S(f)T\psi$ for all $\psi \in D(\Phi_S(f))$. Now, let C be a conjugation on $\mathscr{H}$ and for $f \in \mathscr{H}_C$ define $N(f) = \frac{1}{2}(\Phi_S(f)^2 + \Phi_S(if)^2 - 1)$. Then $N(f) \geq 0$, since $N(f) = d\Gamma((f, \cdot)f)$ and T: $D(N(f)) \to D(N(f))$ with $TN(f)\psi = N(f)T\psi$ for $\psi \in D(N(f))$. Let $\{f_i\}_{i=1}^{\infty}$ be an orthonormal basis for $\mathscr{H}$ with $f_i \in \mathscr{H}_C$ for each i. The reader can check directly that for each $\psi \in D(N)$

$$N\psi = \lim_{n\to\infty} \sum_{i=1}^{n} N(f_i)\psi$$

Thus, $\psi \in Q(N)$, the form domain of N, if and only if $\psi \in \bigcap_{i=1}^{\infty} Q(N(f_i))$ and $\sum_{i=1}^{\infty} (\psi, N(f_i)\psi) < \infty$, and if the sum is finite,

$$(\psi, N\psi) = \sum_{i=1}^{\infty} (\psi, N(f_i)\psi)$$

Since $\Omega_0 \in D(N(f_i))$, $T\Omega_0 \in D(N(f_i))$. Thus, since $N(f_i)\Omega_0 = 0$ for all i we have

$$\sum_{i=1}^{\infty} (T\Omega_0, N(f_i)T\Omega_0) = \sum_{i=1}^{\infty} (T^*T\Omega_0, N(f_i)\Omega_0) = 0$$

Therefore, $T\Omega_0 \in Q(N)$ and $(T\Omega_0, NT\Omega_0) = 0$. Since N is strictly positive on $\{\Omega_0\}^{\perp}$, there exists a constant c so that $T\Omega_0 = c\Omega_0$. Let $\mathscr{P}$ be a polynomial in $\Phi_S(g_1), \ldots, \Phi_S(g_n)$ for some $g_i \in \mathscr{H}$. Then $T(\mathscr{P}\Omega_0) = \mathscr{P}(T\Omega_0) = c\mathscr{P}\Omega_0$. The set of such vectors $\mathscr{P}\Omega_0$ is dense in $\mathscr{F}_s(\mathscr{H})$ by Theorem X.41. Therefore $T = cI$. ∎

Lemma 2 Let $\varphi_m(\cdot)$, $\pi_m(\cdot)$ be the time-zero field and conjugate momentum of the free scalar field of mass m. Then the set

$$\{e^{i\varphi_m(f)}, e^{i\pi_m(f)} \mid f \in \mathscr{S}_{\mathbb{R}}(\mathbb{R}^3)\}$$

is irreducible.

Proof The reader can easily deduce Lemma 2 from Lemma 1 by using the fact that $\mathscr{S}_{\mathbb{R}}(\mathbb{R}^3)$ is dense in $L^2_{\mathbb{R}}(\mathbb{R}^3)$ and the continuity properties of the fields (Theorem X.41d). ∎

Theorem X.46 Let $\varphi_m(\cdot)$, $\pi_m(\cdot)$ be the time-zero field and conjugate momentum of the free scalar field of mass m. Then, if $m_1 \neq m_2$, the representations $\{\exp(i\pi_{m_1}(\cdot)), \exp(i\varphi_{m_1}(\cdot))\}$ and $\{\exp(i\pi_{m_2}(\cdot)), \exp(i\varphi_{m_2}(\cdot))\}$ of the Weyl relations are inequivalent.

Proof Suppose that there exists a unitary map T on $\mathscr{F}_s(L^2(\mathbb{R}^3))$ which satisfies $T\exp(i\varphi_{m_1}(f))T^{-1} = \exp(i\varphi_{m_2}(f))$ and $T\exp(i\pi_{m_2}(f))T^{-1} = \exp(i\pi_{m_1}(f))$ for all $f \in \mathscr{S}(\mathbb{R}^3)$. Let $G_{m_1}(\cdot, \cdot)$ and $G_{m_2}(\cdot, \cdot)$ denote the restrictions of the representations $\Gamma(U_{m_2}(\cdot, \cdot))$ and $\Gamma(U_{m_1}(\cdot, \cdot))$ to the Euclidean group, which is the subgroup of $\mathscr{P}_+^\uparrow$ which leaves the time-zero plane fixed (the semidirect product of the rotation group and the translation group on $\mathbb{R}^3$). For any element $\langle R, a\rangle$ of the Euclidean group, the Poincaré invariance of the fields implies that

$$G_{m_1}(R, a)\varphi_{m_1}(f)G_{m_1}(R, a)^{-1} = \varphi_{m_1}(\langle R, a\rangle f)$$
$$G_{m_2}(R, a)\varphi_{m_2}(f)G_{m_2}(R, a)^{-1} = \varphi_{m_2}(\langle R, a\rangle f)$$

and also the corresponding statements for π_{m_1} and π_{m_2}. From the functional calculus it follows that

$$G_{m_1}(R, a)\exp(i\varphi_{m_1}(f))G_{m_1}(R, a)^{-1} = \exp(i\varphi_{m_1}(\langle R, a\rangle f))$$
$$G_{m_2}(R, a)\exp(i\varphi_{m_2}(f))G_{m_2}(R, a)^{-1} = \exp(i\varphi_{m_2}(\langle R, a\rangle f))$$

and similar statements for π_{m_1} and π_{m_2}. From these relations and the properties of T the reader can quickly check that for each $\langle R, a\rangle$ and each $f \in \mathscr{S}(\mathbb{R}^3)$, $TG_{m_1}(R, a)T^{-1}G_{m_2}(\langle R, a\rangle^{-1})$ commutes with both $\exp(i\pi_{m_2}(f))$ and $\exp(i\varphi_{m_2}(f))$. By Lemma 2 this implies that

$$TG_{m_1}(R, a)T^{-1}G_{m_2}(\langle R, a\rangle^{-1}) = C(R, a)$$

or equivalently

$$TG_{m_1}(R, a)T^{-1} = C(R, a)G_{m_2}(R, a)$$

where $C(R, a)$ is a constant which a priori might depend on R and a. It follows from the above relations that $C(\cdot, \cdot)$ is a one-dimensional representation of the Euclidean group. It is not hard to show (Problem 41) that the identity representation is the only such representation. Thus

$$TG_{m_1}(R, a)T^{-1} = G_{m_2}(R, a)$$

for all $\langle R, a\rangle$ in the Euclidean group. And from this it follows that $T\Omega_0 = \alpha\Omega_0$ since Ω_0 is the unique vector invariant under both G_{m_1} and G_{m_2}. Thus

$$\begin{aligned}(\Omega_0, \varphi_{m_1}(f)\varphi_{m_1}(g)\Omega_0) &= (\Omega_0, T\varphi_{m_1}(f)T^{-1}T\varphi_{m_1}(g)T^{-1}\Omega_0)\\ &= (\Omega_0, \varphi_{m_2}(f)\varphi_{m_2}(g)\Omega_0)\end{aligned}$$

which implies that $(\Omega_0, \varphi_{m_1}(x)\varphi_{m_1}(y)\Omega_0)$ and $(\Omega_0, \varphi_{m_2}(x)\varphi_{m_2}(y)\Omega_0)$ are equal as tempered distributions on $\mathscr{S}(\mathbb{R}^3) \times \mathscr{S}(\mathbb{R}^3)$. But

$$(\Omega_0, \varphi_{m_1}(x)\varphi_{m_1}(y)\Omega_0) = \Delta_+(x - y, m_1^2)$$

and

$$(\Omega_0, \varphi_{m_2}(x)\varphi_{m_2}(y)\Omega_0) = \Delta_+(x - y, m_2^2)$$

and these distributions are *not* equal if $m_1 \neq m_2$. Thus no such T having the indicated properties can exist. Therefore the representations of the Weyl relations are inequivalent. ∎

X.8 Semigroups and their generators

A family of bounded operators $\{T(t) | 0 \leq t < \infty\}$ on a Banach space X is called a **strongly continuous semigroup** if:

(a) $T(0) = I$
(b) $T(s)T(t) = T(s + t)$ for all $s, t \in \mathbb{R}^+$
(c) For each $\varphi \in X$, $t \mapsto T(t)\varphi$ is continuous.

Such semigroups arise naturally in the theory of partial differential equations and in quantum theory; this section is devoted to studying their fundamental properties. We will see that strongly continuous semigroups are the "exponentials," $T(t) = e^{-tA}$, of a certain class of operators. Thus, they provide a generalization of the relationship between unitary groups and self-adjoint operators. In particular, Stone's theorem, the fundamental criterion, the core theorem (Theorem VIII.11), and the Kato–Rellich theorem, all have generalizations to strongly continuous semigroups and their generators. The only important property of self-adjoint operators that does not generalize is the spectral theorem. There is a different class of operators called "spectral operators" for which there is an analogue of the spectral theorem. We give references in the Notes. The theory of semigroups has applications to the study of parabolic and hyperbolic partial differential equations. Throughout this section we use the heat equation to illustrate these applications. More general differential equations are discussed in the Notes.

We begin by studying a special class of semigroups:

Definition A family $\{T(t) | 0 \leq t < \infty\}$ of bounded operators on a Banach space X is called a **contraction semigroup** if it is a strongly continuous semigroup and moreover $\|T(t)\| \leq 1$ for all $t \in [0, \infty)$.

As the reader will see, theorems about general strongly continuous semigroups are easy generalizations of the corresponding theorems for contraction semigroups. Thus, we study the special case first. We then briefly discuss the general theory and conclude the section by studying another special class, holomorphic semigroups.

Let $T(t)$ be a contraction semigroup on a Banach space X. As in the case of unitary groups on Hilbert spaces we obtain the generator of $T(t)$ by differentiation. Set $A_t = t^{-1}(I - T(t))$ and define

$$D(A) = \left\{ \varphi \,\middle|\, \lim_{t \downarrow 0} A_t \varphi \text{ exists} \right\}$$

For $\varphi \in D(A)$, we define $A\varphi = \lim_{t \downarrow 0} A_t \varphi$. Our first goal is to show that $D(A)$ is dense. We use an idea similar to the technique used in the proof of Stone's theorem. For $\varphi \in X$, we set

$$\varphi_s = \int_0^s T(t)\varphi \, dt$$

Since $T(t)$ is strongly continuous, we need only use the Riemann integral.

For any $r > 0$, $T(r)\varphi_s = \int_0^s T(t + r)\varphi \, dt$; thus

$$\begin{aligned} A_r \varphi_s &= -\frac{1}{r} \int_0^s (T(t + r)\varphi - T(t)\varphi) \, dt \\ &= -\frac{1}{r} \int_s^{r+s} T(t)\varphi \, dt + \frac{1}{r} \int_0^r T(t)\varphi \, dt \\ &\xrightarrow[r \downarrow 0]{} -T(s)\varphi + \varphi \end{aligned}$$

Therefore, for each $\varphi \in X$ and $s > 0$, $\varphi_s \in D(A)$. Since $s^{-1}\varphi_s \to \varphi$ as $s \to 0$, A is densely defined. Furthermore, if $\varphi \in D(A)$, then $A_r T(t)\varphi = T(t)A_r \varphi$, so $T(t)$: $D(A) \to D(A)$ and

$$\frac{d}{dt} T(t)\varphi = -AT(t)\varphi = -T(t)A\varphi \tag{X.97}$$

A is also closed, for if $\varphi_n \in D(A)$, $\varphi_n \to \varphi$, and $A\varphi_n \to \psi$, then

$$\begin{aligned} \lim_{r \to 0} A_r \varphi &= \lim_{r \to 0} \lim_{n \to \infty} -\frac{1}{r} (T(r)\varphi_n - \varphi_n) \\ &= \lim_{r \to 0} \lim_{n \to \infty} \frac{1}{r} \int_0^r T(t)A\varphi_n \, dt \qquad \text{(by (X.97))} \\ &= \lim_{r \to 0} \frac{1}{r} \int_0^r T(t)\psi \, dt \\ &= \psi \end{aligned}$$

so $\varphi \in D(A)$ and $A\varphi = \psi$. We have thus proven:

Proposition Let $T(t)$ be a strongly continuous semigroup on a Banach space X and set $A\varphi = \lim_{r\to 0} A_r\varphi$ where $D(A) = \{\varphi \mid \lim_{r\downarrow 0} A_r\varphi \text{ exists}\}$. Then A is closed and densely defined. A is called the **infinitesimal generator** of $T(t)$. We will also say that A generates $T(t)$ and write $T(t) \equiv e^{-tA}$.

It is natural to ask what additional properties the generator of a contraction semigroup possesses. The formal Laplace transform

$$\frac{1}{\lambda + A} = -\int_0^\infty e^{-\lambda t}e^{-tA}\,dt$$

suggests that all μ with $\operatorname{Re}\mu < 0$ are in $\rho(A)$. This is in fact true and the formula holds in the strong sense. For suppose that $\operatorname{Re}\lambda > 0$. Then, since $\|e^{-tA}\| \le 1$,

$$R\varphi = \int_0^\infty e^{-\lambda t}(e^{-tA}\varphi)\,dt$$

defines a bounded linear operator of norm less than or equal to $(\operatorname{Re}\lambda)^{-1}$. Moreover, for $r > 0$,

$$\begin{aligned} A_r R\varphi &= -\frac{1}{r}\int_0^\infty e^{-\lambda t}(e^{-(t+r)A} - e^{-tA})\varphi\,dt \\ &= \left(\frac{1 - e^{\lambda r}}{r}\right)\int_0^\infty e^{-\lambda t}e^{-tA}\varphi\,dt + \frac{e^{r\lambda}}{r}\int_0^r e^{-\lambda t}e^{-tA}\varphi\,dt \end{aligned}$$

so as $r \to 0$, $A_r R\varphi \to \varphi - \lambda R\varphi$. Thus $R\varphi \in D(A)$ and $AR\varphi = \varphi - \lambda R\varphi$ which implies $(\lambda + A)R\varphi = \varphi$. In addition, for $\varphi \in D(A)$ we have $AR\varphi = RA\varphi$ since

$$A\int_0^\infty e^{-\lambda t}e^{-tA}\varphi\,dt = \int_0^\infty e^{-\lambda t}Ae^{-tA}\varphi\,dt = \int_0^\infty e^{-\lambda t}e^{-tA}A\varphi\,dt$$

The first equality follows by approximation with Riemann sums from the facts that $e^{-\lambda t}e^{-tA}\varphi$ and $Ae^{-\lambda t}e^{-tA}\varphi$ are integrable, A is closed. Thus, for $\varphi \in D(A)$, $R(\lambda + A)\varphi = \varphi = (\lambda + A)R\varphi$ which implies that

$$R = (\lambda + A)^{-1}$$

The properties of A which we have derived are also sufficient to guarantee that A generates a contraction semigroup. In fact, we only need information about real positive λ. This theorem (which we generalize later) is the analogue of Stone's theorem for self-adjoint operators.

Theorem X.47a (Hille–Yosida) A necessary and sufficient condition that a closed linear operator A on a Banach space X generate a contraction semigroup is that

(i) $(-\infty, 0) \subset \rho(A)$
(ii) $\|(\lambda + A)^{-1}\| \leq \lambda^{-1}$ for all $\lambda > 0$.

Furthermore, if A satisfies (i) and (ii), then the entire open left half-plane is contained in $\rho(A)$ and

$$(\lambda + A)^{-1}\varphi = -\int_0^\infty e^{-\lambda t}e^{-tA}\varphi \, dt \tag{X.98}$$

for all $\varphi \in X$ and λ with $\operatorname{Re}\lambda > 0$. Finally, if $T_1(t)$ and $T_2(t)$ are contraction semigroups generated by A_1 and A_2 respectively, then $T_2(t) \neq T_1(t)$ for some t implies that $A_1 \neq A_2$.

Proof Since we showed above that conditions (i) and (ii) are necessary and that (X.98) holds, we need only show sufficiency. So, suppose that A is a closed operator on X satisfying (i) and (ii). For $\lambda > 0$, define $A^{(\lambda)} = \lambda - \lambda^2(\lambda + A)^{-1}$. We will show that as $\lambda \to \infty$, $A^{(\lambda)} \to A$ strongly on $D(A)$ and then construct e^{-At} as the strong limit of the semigroups $e^{-tA^{(\lambda)}}$.

For $\varphi \in D(A)$, $A^{(\lambda)}\varphi = \lambda(\lambda + A)^{-1}A\varphi$. Moreover, by (ii),

$$\lambda(\lambda + A)^{-1}\varphi - \varphi = -(\lambda + A)^{-1}A\varphi \xrightarrow[\lambda \to \infty]{} 0$$

By condition (ii) the family $\{\lambda(\lambda + A)^{-1} \mid \lambda > 0\}$ is uniformly bounded in norm, so since $D(A)$ is dense, $\lambda(\lambda + A)^{-1}\psi \to \psi$ for all $\psi \in X$. Thus $A^{(\lambda)}\varphi \to A\varphi$ for all $\varphi \in D(A)$.

Since $A^{(\lambda)}$ is bounded, the semigroups $e^{-tA^{(\lambda)}}$ can be defined by power series. Since

$$\begin{aligned}\|e^{-tA^{(\lambda)}}\| &= \|e^{-\lambda t}e^{+t\lambda^2(\lambda+A)^{-1}}\| \\ &\leq e^{-\lambda t}\sum \frac{t^n\lambda^{2n}}{n!}\|(\lambda + A)^{-1}\|^n \\ &\leq 1\end{aligned}$$

they are contraction semigroups. For all μ, λ, $t > 0$, and all $\varphi \in D(A)$, we have

$$e^{-tA^{(\lambda)}}\varphi - e^{-tA^{(\mu)}}\varphi = \int_0^t \frac{d}{ds}\left(e^{-sA^{(\lambda)}}e^{-(t-s)A^{(\mu)}}\varphi\right) ds$$

so,

$$\begin{aligned}\|e^{-tA^{(\lambda)}}\varphi - e^{-tA^{(\mu)}}\varphi\| &\leq \int_0^t \|e^{-sA^{(\lambda)}}e^{-(t-s)A^{(\mu)}}\| \, \|A^{(\mu)}\varphi - A^{(\lambda)}\varphi\| \, ds \\ &\leq t\|A^{(\mu)}\varphi - A^{(\lambda)}\varphi\|\end{aligned}$$

We have used the fact that $e^{-(t-s)A^{(\mu)}}$ and $e^{-tA^{(\lambda)}}$ commute since $\{A^{(\lambda)}\}_{\lambda>0}$ is a commuting family. Since we have proven above that $A^{(\lambda)}\varphi \to A\varphi$, $\{e^{-tA^{(\lambda)}}\varphi\}$ is Cauchy as $\lambda \to \infty$ for each $t > 0$ and $\varphi \in D(A)$. Since $D(A)$ is dense and the $e^{-tA^{(\lambda)}}$ are uniformly bounded, the same statement holds for all $\varphi \in X$. Now, define $T(t)\varphi = \lim_{\lambda\to\infty} e^{-tA^{(\lambda)}}\varphi$. $T(t)$ is a semigroup of contraction operators since these properties are preserved under strong limits. The above inequality shows that the convergence $e^{-tA^{(\lambda)}}\varphi \to T(t)\varphi$ is uniform for t restricted to a finite interval, so $T(t)$ is strongly continuous since $e^{-tA^{(\lambda)}}$ is. Thus, $T(t)$ is a contraction semigroup.

It remains to show that the infinitesimal generator of $T(t)$, call it $\tilde{A}$, is equal to A. For all t and $\varphi \in D(A)$,

$$e^{-tA^{(\lambda)}}\varphi - \varphi = -\int_0^t e^{-sA^{(\lambda)}}A^{(\lambda)}\varphi \, ds$$

so, since $A^{(\lambda)}\varphi \to A\varphi$, we have

$$T(t)\varphi - \varphi = -\int_0^t T(s)A\varphi \, ds$$

Thus, $\tilde{A}_t\varphi \to A\varphi$ as $t \to 0$. Therefore $D(\tilde{A}) \supset D(A)$ and $\tilde{A} \restriction D(A) = A$. For $\lambda > 0$, $(\lambda + A)^{-1}$ exists by hypothesis and $(\lambda + \tilde{A})^{-1}$ exists by the necessity part of the theorem. Thus $(\lambda + \tilde{A})D(\tilde{A}) = X = (\lambda + A)D(A)$, which implies that $D(\tilde{A}) = D(A)$.

Finally, suppose that $T_1(t)$ and $T_2(t)$ are contraction semigroups so that $T_1(t_0) \neq T_2(t_0)$ for some $t_0 > 0$. Then there is an $\ell \in X^*$ and a $\varphi \in X$ so that $\ell(T_1(t_0)\varphi) \neq \ell(T_2(t_0)\varphi)$. Since (X.98) holds for both $T_1(t)$ and $T_2(t)$, we conclude that $\ell((\lambda + A_1)^{-1}\varphi) \neq \ell((\lambda + A_2)^{-1}\varphi)$ for some λ with $\operatorname{Re}\lambda > 0$ because the ordinary Laplace transform is injective on the bounded functions. Thus, the resolvents of A_1 and A_2 differ, so $A_1 \neq A_2$. ∎

It is possible to construct e^{-tA} in the sufficiency part of Theorem X.47a by using the formula $e^{-tA} = \lim_{n\to\infty}(1 + (t/n)A)^{-n}$ (see Problem 49).

The difficulty in applying Theorem X.47a directly is that it is necessary to construct the resolvent of the closed operator A in order to verify conditions (i) and (ii). It is therefore convenient to have conditions on the operator A itself, that is, we seek an analogue of the symmetry condition and the fundamental criterion condition for self-adjoint operators. To see what these conditions should be, consider the Hilbert space case. If $\varphi \in D(A)$, then the fact that $\|e^{-tA}\varphi\|^2 \leq \|\varphi\|^2$ for all $t > 0$ implies that $(d/dt)\|e^{-tA}\varphi\|^2\big|_{t=0} \leq 0$. On the other hand,

$$\frac{d}{dt}\|e^{-tA}\varphi\|^2\bigg|_{t=0} = -(A\varphi, \varphi) - (\varphi, A\varphi)$$

so we conclude that $\text{Re}\,(A\varphi,\ \varphi) \geq 0$. Thus, we need to generalize the condition $\text{Re}\,(A\varphi, \varphi) \geq 0$ to the Banach space case.

Definition Let X be a Banach space, $\varphi \in X$. An element $\ell \in X^*$ that satisfies $\|\ell\| = \|\varphi\|$, and $\ell(\varphi) = \|\varphi\|^2$ is called a **normalized tangent functional** to φ. By the Hahn–Banach theorem, each $\varphi \in X$ has at least one normalized tangent functional.

Definition A densely defined operator A on a Banach space X is called **accretive** if for each $\varphi \in D(A)$, $\text{Re}(\ell(A\varphi)) \geq 0$ for some normalized tangent functional to φ. A is called **maximal accretive** (or **m-accretive**) if A is accretive and A has no proper accretive extension.

We remark that an accretive operator is closable (Problem 52). The closure of an accretive operator is again accretive, so every accretive operator has a smallest closed accretive extension. We can now state the fundamental criterion.

Theorem X.48 A closed operator A on a Banach space X is the generator of a contraction semigroup if and only if A is accretive and $\text{Ran}(\lambda_0 + A) = X$ for some $\lambda_0 > 0$.

Proof Let e^{-tA} be a contraction semigroup and suppose that ℓ is any normalized tangent functional to $\varphi \in D(A)$. Then $\ell(e^{-tA}\varphi)$ is differentiable and

$$\frac{d}{dt}\,\text{Re}(\ell(e^{-tA}\varphi))\bigg|_{t=0} = -\text{Re}\,\ell(A\varphi)$$

On the other hand

$$|\ell(e^{-tA}\varphi)| \leq \|\ell\|\,\|e^{-tA}\varphi\| \leq \|\varphi\|^2 = \ell(\varphi)$$

for all $t > 0$, so $\text{Re}\,t^{-1}(\ell(e^{-tA}\varphi) - \ell(\varphi)) \leq 0$ for all $t > 0$. Thus,

$$-\text{Re}(\ell(A\varphi)) \leq 0$$

for all normalized tangent functionals to φ, so A is accretive. The fact that $\text{Ran}(I + A) = X$ is a consequence of (i) in Theorem X.47a. This proves necessity.

To show sufficiency, suppose $\lambda > 0$ and A is a closed accretive operator satisfying $\text{Ran}(\lambda_0 + A) = X$, for some $\lambda_0 > 0$. Let ℓ be a normalized tangent

functional to $\varphi \in D(A)$ so that $\mathrm{Re}(\ell(A\varphi)) \geq 0$. Then

$$\begin{aligned}\lambda\|\varphi\|^2 &\leq \lambda\ell(\varphi) + \mathrm{Re}\,\ell(A\varphi)\\ &= \mathrm{Re}\,\ell((\lambda + A)\varphi)\\ &\leq \|\varphi\|\,\|(\lambda + A)\varphi\|\end{aligned}$$

Thus, $\mathrm{Ran}(\lambda + A)$ is closed and $\lambda + A$ has a bounded inverse from $\mathrm{Ran}(\lambda + A)$ to $D(A)$ of norm less than or equal to λ^{-1}. To complete the proof we need only show that $\mathrm{Ran}(\lambda + A)$ is dense. But $\mathrm{Ran}(\lambda + A)$ is dense for $\lambda = \lambda_0$, so the usual perturbation argument (see the proof of Theorem X.1) shows that $\mathrm{Ran}(\lambda + A)$ is dense for all $\lambda > 0$. ∎

Corollary Let A be a closed operator on a Banach space X. Then, if both A and its adjoint A' are accretive, A generates a contraction semigroup.

Proof Suppose that $\mathrm{Ran}(I + A)$ is not dense. Then by the Hahn–Banach theorem there is an $\ell \in X^*$ so that $\ell((I + A)\varphi) = 0$ for all $\varphi \in D(A)$. Thus, $\ell \in D(A')$ and $(I + A')\ell = 0$. So, if μ is any normalized tangent functional to ℓ in X^{**}, $\mu(A'\ell) = -\|\ell\|^2$, which contradicts the assumption that A' is accretive unless $\ell = 0$. Thus, $\mathrm{Ran}(I + A)$ is dense. ∎

Before giving some examples, we make several remarks. First, to prove sufficiency in Theorem X.48, we used only the assumption that there exists at least one normalized tangent functional ℓ for each $\varphi \in D(A)$ with $\mathrm{Re}\,\ell(A\varphi) \geq 0$. From this it followed that $(\lambda + A)^{-1}$ was bounded for each $\lambda > 0$. Using the further assumption that $\mathrm{Ran}(\lambda_0 + A) = X$ we then concluded the proof of sufficiency. However, the necessity part of the argument showed that if A generates a contraction semigroup, then $\mathrm{Re}\,\ell(A\varphi) \geq 0$ for *all* tangent functionals. Thus, in the presence of the assumption $\mathrm{Ran}(I + A) = X$, the condition that $\mathrm{Re}\,\ell(A\varphi) \geq 0$ for one tangent functional (for each $\varphi \in D(A)$) implies $\mathrm{Re}\,\ell(A\varphi) \geq 0$ for all tangent functionals. Secondly, the generators of contraction semigroups are clearly maximal accretive since the condition $\mathrm{Ran}(I + A) = X$ implies that A has no proper accretive extensions. The converse statement, i.e., if A is maximal accretive, then A generates a contraction semigroup, holds in the Hilbert space case but not in the Banach space case (see the Notes and Problem 50). Finally, as in the case of self-adjoint operators, there is a core theorem for the generators of contraction semigroups:

Theorem X.49 Let A be the generator of a contraction semigroup on a Banach space X. Let D be a dense set, $D \subset D(A)$, so that $e^{-tA}\colon D \to D$. Then D is a core for A (i.e., $\overline{A \restriction D} = A$).

Proof Let $\lambda > 0$. We need only show that $\mathrm{Ran}(\lambda + A \restriction D)$ is dense. Suppose not. Then there is a $\ell \in X^*$, $\ell \neq 0$, so that $\ell((\lambda + A)\varphi) = 0$ for all $\varphi \in D$. But, if $\varphi \in D$,

$$\frac{d}{dt}\ell(e^{-tA}\varphi) = \ell(-Ae^{-tA}\varphi) = \lambda\ell(e^{-tA}\varphi)$$

since $e^{-tA}\varphi \in D$. Thus $\ell(e^{-tA}\varphi) = \ell(\varphi)e^{\lambda t}$ which for large enough t contradicts the fact that e^{-tA} is a contraction unless $\ell(\varphi) = 0$. Since D is dense, $\ell(\varphi)$ cannot equal zero for all $\varphi \in D$, so we conclude that $\mathrm{Ran}(\lambda + A \restriction D)$ is dense. ∎

Example 1 Let B be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Then $\|(\mu - B)^{-1}\| \leq |\mathrm{Im}\,\mu|^{-1}$, so the operators $A_1 = iB$ and $A_2 = -iB$ both satisfy the hypotheses of the Hille–Yosida theorem. The contraction semigroups e^{-tA_1}, and e^{-tA_2} are equal to the unitary groups e^{itB} for $t < 0$ and $t > 0$ respectively.

If $B \geq 0$, then B itself satisfies the hypotheses of the Hille–Yosida theorem since $\|(\mu + B)^{-1}\| \leq \mu^{-1}$ for $\mu > 0$ by the functional calculus. Thus, B generates a contraction semigroup e^{-Bt}. Of course, these semigroups can be constructed directly from the functional calculus.

Example 2 (the heat equation on $L^2(\mathbb{R}^n)$) The operator $-\Delta$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R}^n)$ and positive so its closure (which we also denote by $-\Delta$) generates a semigroup $e^{\Delta t}$ on $L^2(\mathbb{R}^n)$. For $f \in L^2(\mathbb{R}^n)$, we define $u(x, t) = e^{\Delta t}f$. Then for all $\varphi \in C_0^\infty(\mathbb{R}^n \times (0, \infty))$,

$$\begin{aligned}
&\int_{\mathbb{R}^{n+1}} \overline{\left(\left(-\frac{\partial}{\partial t} - \Delta\right)\varphi(x, t)\right)} u(x, t)\, dx\, dt \\
&\quad = \int_{\mathbb{R}} \left(\int_{\mathbb{R}^n} \overline{\left(\left(-\frac{\partial}{\partial t} - \Delta\right)\varphi(x, t)\right)} e^{\Delta t} f(x)\, dx \right) dt \\
&\quad = \int_{\mathbb{R}} \left(\int_{\mathbb{R}^n} \overline{\left(e^{\Delta t}\left(-\frac{\partial}{\partial t} - \Delta\right)\varphi(x, t)\right)} f(x)\, dx \right) dt \\
&\quad = \int_{\mathbb{R}} \int_{\mathbb{R}^n} -\frac{\partial}{\partial t}\left[\overline{(e^{\Delta t}\varphi)(x, t)} f(x)\right] dx\, dt \\
&\quad = 0
\end{aligned}$$

so $u(x, t)$ is a weak solution of the heat equation $\partial u(x, t)/\partial t = \Delta u(x, t)$. If $f \in D(\Delta)$, then for each $t > 0$, $u(x, t) \in D(\Delta)$ as a function of x, so in this

case $u(x, t)$ is a classical solution in the sense that $u(x, t)$ is an $L^2(\mathbb{R}^n)$-valued differentiable function of t and $\partial u(x, t)/\partial t = \Delta u(x, t)$. In either case $u(x, t)$ satisfies the initial condition $u(x, 0) = f(x)$ in the sense that $\|u(x, t) - f(x)\|_{L^2(\mathbb{R}^n)} \to 0$ as $t \to 0$. We will see later that for $t > 0$, $u(x, t)$ is in fact infinitely differentiable in x and t for all $f \in L^2(\mathbb{R}^n)$. We remark that since $e^{\Delta t}$ is a contraction semigroup $\|u(x, t)\|_{L^2(\mathbb{R}^n)}$ is a nonincreasing function of t.

Example 3 (the heat equation on $C_\infty(\mathbb{R}^n)$) We denote by $C_\infty(\mathbb{R}^n)$ the continuous functions on $\mathbb{R}^n$ with $f(x) \to 0$ as $|x| \to \infty$. $C_\infty(\mathbb{R}^n)$ is a Banach space under the sup norm. We define $-\Delta$ as the closure of the operator $\varphi \to -\Delta\varphi$ on $\mathscr{S}(\mathbb{R}^n)$. We will show that $-\Delta$ satisfies the hypotheses of Theorem X.48. Let $\varphi \in \mathscr{S}(\mathbb{R}^n)$. Then there is a point x_0 so that $|\varphi(x_0)| = \sup_{x \in \mathbb{R}^n} |\varphi(x)|$. Let $\ell_\varphi = \overline{\varphi(x_0)}\delta_{x_0}$. Then $\ell_\varphi \in C_\infty(\mathbb{R}^n)^*$, $\|\ell_\varphi\| = |\varphi(x_0)| = \|\varphi\|$, and $\ell(\varphi) = |\varphi(x_0)|^2 = \|\varphi\|^2$, so ℓ is a normalized tangent functional to φ. Further,

$$\begin{aligned} \operatorname{Re}(\ell_\varphi(-\Delta\varphi)) &= \operatorname{Re}\,\overline{\varphi(x_0)}(-\Delta\varphi(x_0)) \\ &= |\nabla\varphi(x_0)|^2 - \tfrac{1}{2}\Delta|\varphi(x_0)|^2 \\ &\geq 0 \end{aligned}$$

because $\Delta|\varphi(x_0)|^2 \leq 0$ since $|\varphi(x)|^2$ has its maximum at x_0. This shows that $-\Delta \upharpoonright \mathscr{S}(\mathbb{R}^n)$ is accretive, and thus its closure is accretive. Moreover, if $g \in \mathscr{S}(\mathbb{R}^n)$, $\widehat{(1 + k^2)^{-1}\hat{g}} \in \mathscr{S}(\mathbb{R}^n) \subset D(-\Delta)$ and $(I - \Delta)\widehat{(1 + k^2)^{-1}\hat{g}} = g$ so $\operatorname{Ran}(I - \Delta)$ contains $\mathscr{S}(\mathbb{R}^n)$ which is dense in $C_\infty(\mathbb{R}^n)$. Since $\operatorname{Ran}(I - \Delta)$ is closed, we conclude that $\operatorname{Ran}(I - \Delta) = C_\infty(\mathbb{R}^n)$. Thus, $-\Delta$ is accretive and satisfies $\operatorname{Ran}(I - \Delta) = C_\infty(\mathbb{R}^n)$, so by Theorem X.48, $-\Delta$ generates a contraction semigroup $e^{\Delta t}$ on $C_\infty(\mathbb{R}^n)$. As in Example 2, it may be shown that for $f \in C_\infty(\mathbb{R}^n)$, $u(x, t) = e^{\Delta t}f$ is a weak solution of the heat equation. We will see later that $u(x, t)$ is in fact a strict solution. $u(x, t)$ satisfies the initial condition $u(x, 0) = f(x)$ in the sense that

$$\sup_{x \in \mathbb{R}^n} |u(x, t) - f(x)| \to 0 \qquad \text{as} \quad t \to 0$$

Since $e^{\Delta t}$ is a contraction semigroup, $\max_{x \in \mathbb{R}^n} |u(x, t)|$ is a nonincreasing function of t. This reflects the intuitive notion that the maximum temperature should decrease as the heat diffuses.

Since $e^{t\Delta}$ has an explicit kernel, we could have analyzed Examples 2 and 3 by "direct" methods. The advantage of the abstract theory is in cases where there is no explicit solution available. See, for instance, Example 4, p. 245.

There is also a perturbation theorem for generators of contraction semigroups analogous to the Kato–Rellich theorem. We first prove a lemma which we later strengthen.

Lemma Let A be the generator of a contraction semigroup on a Banach space X. Suppose that B is an accretive operator, with $D(B) \supset D(A)$, and

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\|$$

for some b, some $a < \frac{1}{2}$, and all $\varphi \in D(A)$. Then $A + B$ (defined on $D(A)$) is a closed accretive operator and generates a contraction semigroup.

Proof The idea of the proof is the same as the proof of Theorem X.12. Let $\lambda > 0$. Then $\|A(\lambda + A)^{-1}\| = \|\lambda(\lambda + A)^{-1} - 1\| \leq 2$. Thus for $\varphi \in D(A)$,

$$\|B(\lambda + A)^{-1}\varphi\| \leq a\|A(\lambda + A)^{-1}\varphi\| + b\|(\lambda + A)^{-1}\varphi\|$$

$$\leq \left(2a + \frac{b}{\lambda}\right)\|\varphi\|$$

Thus, for λ sufficiently large, $\|B(\lambda + A)^{-1}\| < 1$. Therefore, since

$$\mathrm{Ran}(\lambda + \mathrm{A}) = X$$

and

$$(\lambda + A + B) = (I + B(\lambda + A)^{-1})(\lambda + A)$$

we conclude that $\mathrm{Ran}(\lambda + A + B) = X$. Since A generates a contraction semigroup, we know that $\mathrm{Re}(\ell(A\varphi)) \geq 0$ for *every* normalized tangent functional to φ. Thus $A + B$ is accretive and generates a contraction semigroup. ∎

Theorem X.50 Let A and C be accretive operators on a Banach space X. Suppose that there is a dense set D, $D \subset D(A)$, $D \subset D(C)$, and an $a \in [0, 1)$ so that

$$\|(A - C)\varphi\| \leq a(\|A\varphi\| + \|C\varphi\|) + b\|\varphi\|$$

for some b and all $\varphi \in D$. Then

(a) $\bar{A}$ generates a contraction semigroup if and only if $\bar{C}$ does.
(b) $D(\overline{A \restriction D}) = D(\overline{C \restriction D})$.

Proof To prove (a), one need only show that $\mathrm{Ran}(\lambda_0 + A)$ is dense for some $\lambda_0 > 0$ if and only if $\mathrm{Ran}(\mu_0 + C)$ is dense for some $\mu_0 > 0$. The proof is exactly the same as the proof of Theorem X.13 except that we choose α' so that $2a\alpha'/(1 - a) < \frac{1}{2}$ so we can use the lemma. As before, part (b) is left to the reader. ∎

Corollary Let A and B satisfy all the hypotheses of the lemma except that the condition $a < \frac{1}{2}$ is replaced by $a < 1$. Then the conclusion of the lemma holds.

As in the case of self-adjoint operators we have a product formula:

Theorem X.51 (the Trotter product formula) Let A and B be the generators of contraction semigroups on a Banach space X. Suppose that the closure of $(A + B) \restriction D(A) \cap D(B)$ generates a contraction semigroup on X. Then, for all $\varphi \in X$,

$$e^{-t\overline{(A+B)}}\varphi = \lim_{n\to\infty} (e^{-tA/n}e^{-tB/n})^n\varphi$$

In the case where $D = D(A) \cap D(B)$ and $(A + B) \restriction D$ is closed, the proof of Theorem X.41 is exactly the same as the proof given in Theorem VIII.30. For the general case, see the references in the Notes.

Example 4 (the heat equation with sources and sinks proportional to the temperature) Let $q(x)$ be a bounded ($|q(x)| < M$), real-valued continuous function on $\mathbb{R}^n$. The differential equation

$$\frac{\partial}{\partial t} u(x, t) - \Delta u(x, t) = -q(x)u(x, t) \tag{X.99}$$

corresponds to the physical situation where a source adds (if $q(x) \leq 0$) or subtracts (if $q(x) \geq 0$) heat at the point x proportionally to the local temperature at x at time t. Our previous discussion suggests that we consider the operator

$$A = -\Delta + q(x)$$

on $L^2(\mathbb{R}^n)$ and $C_\infty(\mathbb{R}^n)$. Since $q(x)$ is bounded by M as an operator on $L^2(\mathbb{R}^n)$, the Kato–Rellich theorem immediately implies that A is self-adjoint on $D(-\Delta)$ and bounded below by $-M$. Thus, e^{-tA} can be defined by using the functional calculus and if $f \in D(-\Delta)$, then $u(x, t) = e^{-At}f$ satisfies (X.99) with initial conditions $u(x, 0) = f(x)$.

In the case of $C_\infty(\mathbb{R}^n)$ we use the corollary to Theorem X.50, the Banach space analogue of the Kato–Rellich theorem. Suppose first that $q(x) \geq 0$. Then multiplication by $q(x)$ is a bounded accretive operator on $D(-\Delta) \subset C_\infty(\mathbb{R}^n)$ for we can use the same normalized tangent functionals, ℓ_φ as in Example 3, and find that $\ell_\varphi(q\varphi) = q(x_0)|\varphi(x_0)|^2 \geq 0$. Thus, by the corollary to Theorem X.50, A is a closed accretive operator on $D(-\Delta)$.

As before, $u(x, t) = e^{-At}f$ satisfies (X.99) weakly and $\|u(x, t) - f(x)\|_\infty \to 0$ as $t \to \infty$.

If q is negative at any point, then multiplication by q is *not* accretive on $C_\infty(\mathbb{R}^n)$. This is natural since we would only expect e^{-tA} to be a contraction semigroup if $q(x) \geq 0$ (i.e., if heat is only absorbed but not added). But, we can easily surmount this difficulty by defining $A_M = -\Delta + q(x) + M$ on $D(-\Delta)$. Since $q(x) + M \geq 0$, $q(x) + M$ is a bounded accretive operator, and we can apply the corollary to construct the contraction semigroup e^{-tA_M}. We now set $T(t) = e^{tM}e^{-tA_M}$. Then $T(t)$ is a strongly continuous semigroup and for each $f \in D(-\Delta)$, $u(x, t) = T(t)f$ satisfies (X.99) weakly.

Intuitively, the solution of the heat equation should be positivity preserving, i.e., if $u(x, 0) \geq 0$ a.e., then $u(x, t) \geq 0$ a.e. [x] for each $t > 0$. In Problem 53, the reader is asked to show that $e^{\Delta t}$ is positivity preserving on $L^2(\mathbb{R}^n)$. Since $e^{-tq(x)} \geq 0$ for all x, $(e^{\Delta t/n}e^{-tq(x)/n})^n f \geq 0$ if $f \geq 0$. By the Trotter product formula

$$(e^{\Delta t/n}e^{-tq(x)/n})^n f \xrightarrow[n \to \infty]{L^2} e^{-t(-\Delta + q)}f$$

so we must have $e^{-t(-\Delta+q)}f \geq 0$ a.e. A similar use of Trotter's formula shows that $T(t) = e^{tM}e^{-t(-\Delta+q+M)}$ is positivity preserving on $C_\infty(\mathbb{R}^n)$ (Problem 54).

The construction of $e^{-(-\Delta+q)t}$ in Example 4, in the case where $q \leq 0$, shows that strongly continuous semigroups which are not contraction semigroups arise naturally. So we will now show how the results for contraction semigroups can be easily generalized. Let $T(t)$ be a strongly continuous semigroup and let $\alpha > 0$. Since $t \mapsto T(t)\varphi$ is continuous and $[0, \alpha]$ is compact, the set $\{\|T(t)\varphi\|, 0 \leq t \leq \alpha\}$ is bounded. Thus, the uniform boundedness principle (Theorem III.9) implies that there is an M so that $\|T(t)\| \leq M$ for all $t \in [0, \alpha]$. Now let $t \in (0, \infty)$. Then we can write $t = n\alpha + \tau$, where $\tau \in [0, \alpha]$. Thus, by the semigroup property

$$\|T(t)\| = \|T(\alpha)^n T(\tau)\| \leq M^{n+1} \leq Me^{\omega t}$$

where $\omega = \alpha^{-1} \log M$. Therefore, all strongly continuous semigroups are exponentially bounded. The inf of the numbers ω so that there is an M with $\|T(t)\| \leq Me^{\omega t}$ is denoted by ω_0 and called the **type** of the semigroup (see Problem 51). We define the **generator** A of $T(t)$ in exactly the same way as for contraction semigroups. As before A is closed and an

argument almost identical to that given before Theorem X.47a shows that if $\lambda > \omega_0$, then $-\lambda \in \rho(A)$ and

$$(\lambda + A)^{-1}\varphi = \int_0^\infty e^{-\lambda t} T(t)\varphi \, dt$$

for all $\varphi \in X$. Thus, if $\omega > \omega_0$ and $\lambda > \omega$,

$$\begin{aligned} \|(\lambda + A)^{-n}\varphi\| &= \left\| \frac{(-1)^n}{n!} \left(\frac{d}{d\lambda}\right)^n (\lambda + A)^{-1}\varphi \right\| \\ &\leq \frac{1}{n!} \left(\int_0^\infty t^n e^{-\lambda t} M e^{\omega t} \, dt \right) \|\varphi\| \\ &= \frac{M\|\varphi\|}{(\lambda - \omega)^n} \end{aligned}$$

Conversely, a few minor changes in the proof of Theorem X.47a show that these conditions are also sufficient for A to generate a strongly continuous semigroup (Problem 55). Thus, we have:

Theorem X.47b (the Hille–Yosida–Phillips theorem) A necessary and sufficient condition for a closed operator A on a Banach space X to generate a strongly continuous semigroup is that

(i) There is an $\omega > 0$ so that each $\lambda > \omega$ is in $\rho(A)$.
(ii) There is an M so that

$$\|(\lambda + A)^{-n}\| \leq \frac{M}{(\lambda - \omega)^n}$$

for all $\lambda > \omega$ and all positive integers n.

In this case we have $\|e^{-tA}\| \leq Me^{\omega t}$ for all $t > 0$ and

$$\|(\lambda + A)^{-1}\| \leq \frac{M}{\mathrm{Re}(\lambda - \omega)}$$

for all λ so that $\mathrm{Re}(\lambda - \omega) > 0$.

Our last topic in this section is the theory of bounded holomorphic semigroups. To see what we are after, consider first the case of a positive self-adjoint operator A in a Hilbert space $\mathscr{H}$. The vector-valued function $e^{-tA}\varphi$ can be analytically continued to the right-half plane by using the functional calculus. This suggests:

Definition Let $\theta \in (0, \pi/2]$. A strongly continuous bounded semigroup $T(t)$, $t > 0$ on a Banach space X is called a **bounded holomorphic semigroup of angle** θ if:

(i) $T(t)$ is the restriction to the positive real axis of an analytic family of operators $T(z)$ in the open sector $S_\theta = \{z \mid |\arg z| < \theta\}$ which obeys $T(z + z') = T(z)T(z')$ for all $z, z' \in S_\theta$.

(ii) For each $\theta_1 < \theta$, $T(z)$ is uniformly bounded in the sector S_{θ_1} and $T(z)\varphi \to \varphi$ if $z \to 0$ in S_{θ_1} for all $\varphi \in X$.

If A is the infinitesimal generator of $T(t)$, we write $T(z) = e^{-zA}$.

We can easily derive several properties of the generator A of a bounded holomorphic semigroup of angle θ. For each $0 < \eta < \theta$, $e^{-(re^{i\eta})A}$ is a bounded strongly continuous semigroup (as a function of r). It is clear that its generator is $e^{i\eta}A$, so the spectrum of $e^{i\eta}A$ must be contained in the right half-plane. Since this is true for all η satisfying $0 \leq |\eta| < \theta$, we conclude that

$$\sigma(A) \subset \overline{S}_{\pi/2-\theta} \equiv \left\{ z \,\middle|\, |\arg z| \leq \frac{\pi}{2} - \theta \right\} \tag{X.100}$$

Furthermore, for each $\theta_1 < \theta$, $e^{-(re^{i\eta})A}$ is uniformly bounded (say by M_1) for all $r > 0$ and all η with $|\eta| \leq \theta_1$. Thus, by Theorem X.47b,

$$\|(\lambda + e^{i\eta}A)^{-1}\| \leq \frac{M_1}{\mathrm{Re}(\lambda)}$$

for all λ with $\mathrm{Re}\,\lambda > 0$. It follows that, given $\theta_1 < \theta$,

$$\|(z + A)^{-1}\| \leq \frac{M_1}{\mathrm{dist}(z, \overline{S}_{\pi/2-\theta_1})} \tag{X.101}$$

for all $z \in \mathbb{C} \backslash \overline{S}_{\pi/2-\theta_1}$ where M_1 depends on θ_1.

In fact, these conditions are also sufficient:

Theorem X.52 A closed operator A on a Banach space X is the generator of a bounded holomorphic semigroup of angle $\theta \leq \pi/2$ if and only if A satisfies conditions (X.100) and (X.101).

Proof We have already proven necessity. We remark that we could prove sufficiency by the same method as in the Hille–Yosida theorem if we had the stronger hypothesis

$$\|(z + A)^{-n}\| \leq \frac{M_1}{(\mathrm{dist}(z, \overline{S}_{\pi/2-\theta_1}))^n}, \qquad n = 1, 2, \ldots \tag{X.101a}$$

instead of (X.101). In most applications, one can verify (X.101a), but the proof of the general case is instructive. The idea of the proof is to use a generalization of the Dunford functional calculus (see Problem 1 and the notes in Chapter VII) to define a semigroup which we then show has the right properties. Let $0 < \theta_2 < \theta_1 < \theta$ and let Γ be the path indicated in Figure X.5. We define

$$T(z) \equiv -\frac{1}{2\pi i}\int_{\Gamma} e^{-\lambda z}(\lambda - A)^{-1}\, d\lambda \tag{X.102}$$

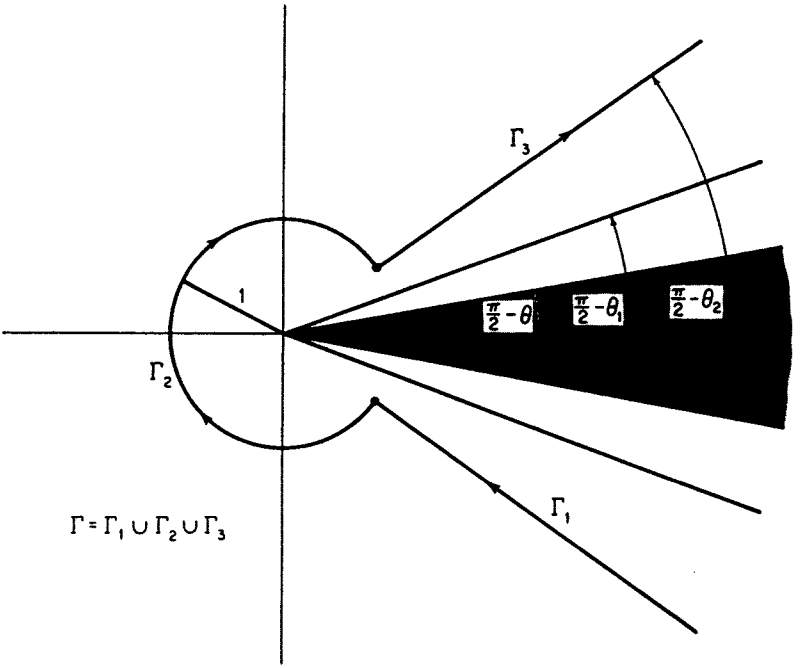


FIGURE X.5 The curve Γ.

for all $z \in S_{\theta_2} = \{z \,|\, |\arg z| < \theta_2\}$. Since $\sigma(A) \subset \bar{S}_{\pi/2-\theta}$, $(\lambda - A)^{-1}$ is well defined on Γ. Moreover, for $\lambda \in \Gamma_1 \cup \Gamma_3$, $\mathrm{Re}(z\lambda) = c(z)|\lambda|$ where $c(z) = |z|\cos(\arg z + \pi/2 - \theta_2)$, so for $z \in S_{\theta_2}$ the integral converges and $\|T(z)\|$ is uniformly bounded in the region

$$R_{\varepsilon,\delta} = \{z \,|\, |z| \geq \delta,\ |\arg z| \leq \theta_2 - \varepsilon\}$$

for each $\varepsilon, \delta > 0$. On the other hand if $0 < |z| \leq \delta$ and $|\arg z| \leq \theta_2 - \varepsilon$, then making the change of variables $\zeta = |z|\lambda$, we find

$$T(z) = \int_{\Gamma'} e^{-\zeta z/|z|} \left(\frac{\zeta}{|z|} - A \right)^{-1} \frac{d\zeta}{|z|}$$

(see Figure X.6)

$$= \int_{\Gamma} e^{-\zeta z/|z|} \left(\frac{\zeta}{|z|} - A \right)^{-1} \frac{d\zeta}{|z|}$$

(by the Cauchy integral formula and (X.101)).

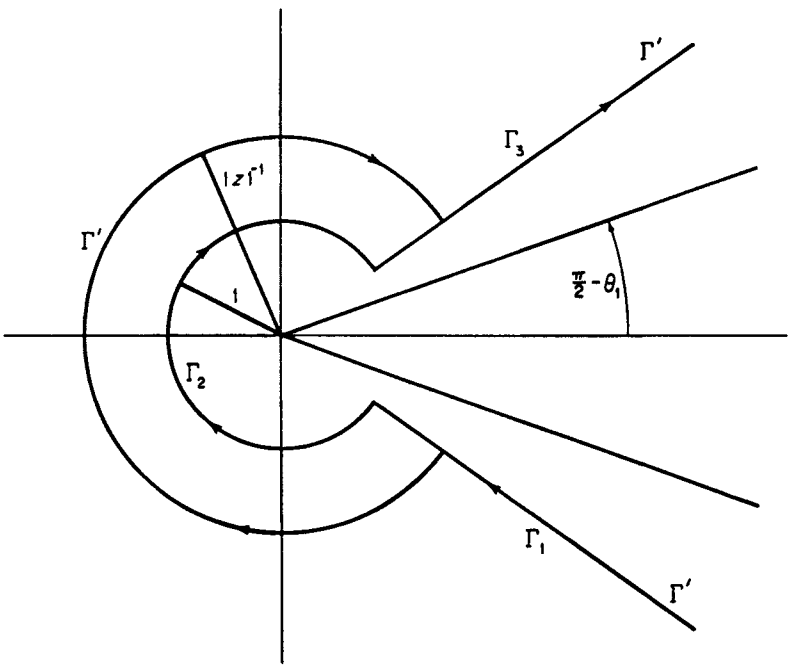


FIGURE X.6 The curve Γ'.

Since for $\zeta \in \Gamma$, $\operatorname{dist}(\zeta/|z|, \bar{S}_{\pi/2-\theta_1}) = |z|^{-1} \operatorname{dist}(\zeta, \bar{S}_{\pi/2-\theta_1})$,

$$\|e^{-zA}\| \leq \int_{\Gamma_1 \cup \Gamma_3} e^{-|\zeta|(1-\cos(\pi/2-\varepsilon))} M_1 \, d\zeta + C$$

$$\leq C_1 \qquad \text{(independently of } z\text{)}$$

so $T(z)$ is uniformly bounded in the sector $R_{\varepsilon,0} = \bar{S}_{\theta_2-\varepsilon}$. Furthermore, $T(z)$ is an analytic operator-valued function in S_{θ_2} since we may differentiate under the integral sign.

To prove that $T(z)$ is a semigroup, we proceed as follows. Let Γ'' be the curve Γ shifted to the left by two units. Then by Cauchy's theorem and (X.101), the definition of $T(z)$ is independent of whether we use Γ or Γ'' to define $T(z)$. Let $z, z' \in S_{\theta_2}$. Then, using Fubini's theorem, the first resolvent formula, and the Cauchy integral formula, we find

$$\begin{aligned} T(z)T(z') &= \left(\frac{1}{2\pi i}\right)^2 \int_\Gamma \int_{\Gamma''} e^{-\lambda z - \mu z'}(\lambda - A)^{-1}(\mu - A)^{-1}\, d\mu\, d\lambda \\ &= \left(\frac{1}{2\pi i}\right)^2 \int_\Gamma \int_{\Gamma''} e^{-\lambda z - \mu z'}(\mu - \lambda)^{-1}((\lambda - A)^{-1} - (\mu - A)^{-1})\, d\mu\, d\lambda \\ &= -\frac{1}{2\pi i}\int_\Gamma e^{-\lambda(z+z')}(\lambda - A)^{-1}\, d\lambda \\ &= T(z + z'). \end{aligned}$$

Now, suppose that $z \to 0$ in the sector $\bar{S}_{\theta_2 - \varepsilon}$ and $\varphi \in D(A)$. Then

$$\begin{aligned} T(z)\varphi - \varphi &= -\frac{1}{2\pi i}\int_\Gamma (e^{-\lambda z}(\lambda - A)^{-1} - e^{-\lambda z}\lambda^{-1})\varphi\, d\lambda \\ &= -\frac{1}{2\pi i}\int_\Gamma e^{-\lambda z}\lambda^{-1}(\lambda - A)^{-1}A\varphi\, d\lambda \\ &\xrightarrow[z\to 0]{} -\frac{1}{2\pi i}\int_\Gamma \lambda^{-1}(\lambda - A)^{-1}A\varphi\, d\lambda \qquad \text{(by the dominated convergence Theorem and (X.101))} \\ &= 0 \qquad \text{(by Cauchy's theorem, (X.100), and (X.101))} \end{aligned}$$

Since the $T(z)$ are uniformly bounded. $T(z)\varphi \to \varphi$ for all $\varphi \in X$. Thus, $T(z)$ is a strongly continuous semigroup in $\bar{S}_{\theta_2 - \varepsilon}$, in particular $T(t)$ is strongly continuous for $t > 0$.

Let $\varphi \in X$. Then as remarked above, we may differentiate under the integral sign to obtain

$$\begin{aligned} \frac{d}{dz}T(z)\varphi &= -\frac{1}{2\pi i}\int_\Gamma e^{-\lambda z}(-\lambda)(\lambda - A)^{-1}\varphi\, d\lambda \\ &= -\frac{1}{2\pi i}\int_\Gamma e^{-\lambda z}(-\varphi - A(\lambda - A)^{-1}\varphi)\, d\lambda \\ &= -\frac{1}{2\pi i}\int_\Gamma e^{-\lambda z}(-A(\lambda - A)^{-1}\varphi)\, d\lambda \qquad \text{(Cauchy's theorem)} \\ &= -A\left[-\frac{1}{2\pi i}\int_\Gamma e^{-\lambda z}(\lambda - A)^{-1}\varphi\, d\lambda\right] \qquad \text{(since } A \text{ is closed)} \\ &= -AT(z)\varphi \end{aligned}$$

Thus, $T(z)$: $X \to D(A)$ and $-AT(z)\varphi = T'(z)\varphi$. Further, if $\varphi \in D(A)$, the same calculation shows that $T'(z)\varphi = -T(z)A\varphi$. Thus, the vector-valued function $T(t)\varphi$ has a uniformly bounded derivative for $t > 0$ so

$$\begin{aligned}\frac{T(t)\varphi - \varphi}{t} &= \frac{1}{t}\int_0^t T'(s)\varphi \, ds \\ &= \frac{1}{t}\int_0^t -AT(s)\varphi \, ds \\ &\xrightarrow[t\to 0]{} -A\varphi\end{aligned}$$

Thus, the generator of $T(t)$ extends A, but since $T(t)$: $D(A) \to D(A)$, Theorem X.49 implies that A itself generates $T(t)$.

Since θ_2 may be taken as close to θ_1 as we like and $\varepsilon > 0$ was arbitrary, we have proven the theorem. ∎

Corollary 1 Let q be a strictly m-accretive form on a Hilbert space $\mathscr{H}$ so that $\varphi \in Q(q)$ implies $|\arg[q(\varphi, \varphi)]| \leq \theta$ where $\theta < \pi/2$. Then the associated strictly m-accretive operator (given in Theorem VIII.16) generates a bounded holomorphic semigroup of angle $\pi/2 - \theta$.

Proof The corollary follows immediately from Theorem VIII.17 and the theorem above. ∎

Corollary 2 Let A be the generator of a bounded holomorphic semigroup of angle θ, $\theta > 0$. Then for each integer $m > 0$ and each $\varphi \in X$, $e^{-tA}\varphi \in D(A^m)$ and $\|A^m e^{-tA}\varphi\| \leq C\|\varphi\|/|t|^m$ for all $t > 0$ (C depends on A and m but not on φ).

The proof of this corollary just uses the representation (X.102), the formula $T'(z) = -AT(z)$, and manipulations similar to those in the theorem. The details are left as Problem 58.

The notion of bounded holomorphic semigroup can be generalized in the same way that we generalized the notion of contraction semigroup. A strongly continuous semigroup $T(t)$ on a Banach space X is called a **holomorphic semigroup of angle** θ if $T(t)$ satisfies all the properties of a bounded holomorphic semigroup of angle θ except that it is not required to be uniformly bounded in sectors $\bar{S}_{\theta_1}$, $\theta_1 < \theta$. If $T(t)$ is a holomorphic semigroup of angle θ, then for each $\theta_1 < \theta$, and $\varphi \in X$, $\|T(z)\varphi\|$ is bounded in

$$\tilde{R}_{1,\theta_1} = \{z \,|\, |\arg z| \leq \theta_1, |z| \leq 1\}$$

so by the uniform boundedness principle, $\|T(z)\|$ is bounded in $\tilde{R}_{1,\theta_1}$. By using the semigroup property as above, one concludes from this that there are constants M, $\omega > 0$ so that

$$\|T(z)\| \leq Me^{\omega|z|}$$

for all $z \in \tilde{S}_{\theta_1}$. Therefore, $e^{-\omega z}T(z)$ is a bounded holomorphic semigroup of angle θ_1. Notice that this is true for all $\theta_1 < \theta$ but ω will in general depend on θ_1. This characterization, Theorem X.52, and Corollary 2 above immediately yield:

Theorem X.53 A closed operator A on a Banach space X is the generator of a holomorphic semigroup of angle θ if and only if for all $\theta_1 < \theta$ there exist constants M, $\omega > 0$ so that $\lambda \notin \tilde{S}_{\pi/2-\theta_1}$ implies that $\lambda - \omega \in \rho(A)$ and

$$\|(A - (\lambda - \omega))^{-1}\| \leq \frac{M}{\operatorname{dist}(\lambda, \tilde{S}_{\pi/2-\theta_1})}$$

Furthermore, there exist constants M_0, $\omega_0 > 0$, so that for all $\varphi \in X$,

$$e^{-tA}\varphi \in \bigcap_{m=1}^{\infty} D(A^m) \qquad \text{and} \qquad \|A^m e^{-tA}\varphi\| \leq \frac{M_0 e^{\omega_0 t}\|\varphi\|}{t^m}$$

for all $t > 0$.

The proof of the following theorem closely parallels the proofs of Theorems X.12 and X.50 and is left to the reader (Problem 56).

Theorem X.54 Suppose that A is the generator of a holomorphic semigroup of angle θ on a Banach space X. Let B be a linear operator on X so that:

(i) $D(B) \supset D(A)$
(ii) For all $a > 0$, there is a $b > 0$ so that for all φ in $D(A)$

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\|$$

Then $A + B$ on $D(A)$ is the generator of a holomorphic semigroup of angle θ.

To illustrate some of the concepts we have introduced and to show the use of holomorphic semigroups we discuss an example.

Example 5 (smoothness of solutions of the heat equation) We have previously shown (in Section IX.7) that the semigroup $e^{t\Delta}$ on $L^2(\mathbb{R}^n)$ may be represented by the formula

$$(e^{t\Delta}f)(x) = (4\pi t)^{-n/2}\int_{\mathbb{R}^n} e^{-|x-y|^2/4t} f(y)\,dy$$

By explicit computation, this formula also defines a strongly continuous semigroup on $C_\infty(\mathbb{R})$ whose infinitesimal generator on $\mathscr{S}(\mathbb{R})$ is $-\Delta$. Thus this is a representation for the semigroup $e^{t\Delta}$ on $C_\infty(\mathbb{R})$ which we constructed in Example 3.

For any $z \in \mathbb{C}$ with Re $z > 0$, we define $e^{z\Delta}$ on $C_\infty(\mathbb{R}^n)$ by

$$(e^{z\Delta}f)(x) = (4\pi z)^{-n/2}\int_{\mathbb{R}^n} e^{-|x-y|^2/4z} f(y)\,dy$$

where we take the 1/2 root with the smallest argument. The reader can check by explicit computation (Problem 57) that $z \to e^{z\Delta}$ is an analytic operator-valued function for Re $z > 0$, that the semigroup property holds, and that if $z \to 0$ in $\bar{S}_\theta$, $|\theta| < \pi/2$, then $e^{z\Delta}f \to f$. Furthermore,

$$\|e^{z\Delta}\| = \|(4\pi z)^{-n/2}e^{-|x|^2/4z}\|_1 = \frac{|z|}{\text{Re } z}$$

so $e^{z\Delta}$ is a bounded holomorphic semigroup of angle $\pi/2$. Notice that if $z = te^{i\theta}$, $0 < |\theta| < \pi/2$, then $e^{te^{i\theta}\Delta}$ provides an example of a bounded semigroup that is not a contraction semigroup.

Suppose that $q(x)$ is a bounded continuous function. Then, by Theorem X.54, $-\Delta + q$, with domain $D(-\Delta)$, generates a holomorphic semigroup of angle $\pi/2$ on $C_\infty(\mathbb{R}^n)$. Further, for any $f \in C_\infty(\mathbb{R}^n)$, $e^{t(\Delta-q)}f \in \bigcap_{m=1}^\infty D((-\Delta+q)^m)$. If we suppose in addition that q is infinitely differentiable with bounded derivatives, then we can show that $e^{t(\Delta-q)}f$ is a C^∞ function of x for each $t > 0$. For let $\varphi \equiv e^{t(\Delta-q)}f$. Then $\varphi \in D((-\Delta+q)) = D(\Delta)$. Further, $\varphi \in D((-\Delta+q)^2)$, so $-\Delta\varphi + q\varphi \in D(\Delta)$. Since $\varphi \in D(\Delta)$, $\nabla\varphi$ is in $C_\infty(\mathbb{R}^n)$ by Problem 57b, and thus $q\varphi \in D(\Delta)$. It follows that $\Delta\varphi \in D(\Delta)$. Continuing in this way we prove that $\Delta^m\varphi \in D(\Delta)$ for all m. In particular, $\Delta^m\varphi$ is continuous for all m, so by Sobolev's lemma (Theorem IX.24) φ is a C^∞ function of x.

A similar proof shows that for $f \in L^2$, $e^{t(\Delta-q)}f$ is C^∞ in x for each $t > 0$. In this case we can conclude that $e^{t(\Delta-q)}f \in \bigcap_{m=1}^\infty D((-\Delta+q)^m)$ directly from the spectral theorem, so we do not need Theorem X.53.

By a simple argument using Sobolev's lemma and Theorem X.53, one can see that under the same hypotheses, the solutions,

$$u(x, t) = (e^{t(\Delta - q)}f)(x)$$

are C^∞ *jointly* in x and t for $t > 0$.

As a final example of the theory of holomorphic semigroups, we will investigate a class of operators which arise in the next section and later. Let $\langle M, \mu\rangle$ be a measure space with $\mu(M) = 1$ and let A be a positive self-adjoint operator on $L^2(M, d\mu)$. Since $L^2 \subset L^p$ for all $1 \le p \le 2$, the contraction semigroup e^{-tA} is a densely defined map of L^p into L^p, $1 \le p \le 2$. The question naturally arises: Under what conditions can e^{-tA} be extended to a contraction semigroup on L^p.

Definition Let $\langle M, \mu\rangle$ be a σ-finite measure space and let A be a positive self-adjoint operator on $L^2(M, d\mu)$. We will call e^{-tA} an **L^p-contractive semigroup** if $\|e^{-tA}\varphi\|_p \le \|\varphi\|_p$ for all $\varphi \in L^2 \cap L^p$, *all* $p \in [1, \infty]$, and all $t > 0$. If the map $t \mapsto e^{-tA}$ is strongly continuous for all $p < \infty$ we will call e^{-tA} a **continuous** L^p-contractive semigroup.

Theorem X.55 Let $\langle M, \mu\rangle$ be a measure space with $\mu(M) = 1$ and A a positive self-adjoint operator on $L^2(M, d\mu)$. Then

(a) If e^{-tA} is positivity preserving and $e^{-tA}1 = 1$, then e^{-tA} is an L^p-contractive semigroup.

(b) Every L^p-contractive semigroup is automatically continuous. Moreover, $\mathrm{Ker}(e^{-tA} \restriction L^p) = \{0\}$ for all $p > 1$ and $\mathrm{Ran}(e^{-tA} \restriction L^q)$ is dense in L^q for all $q < \infty$.

(c) Under the hypotheses of (a), for $1 < p < \infty$, e^{-tA} is a bounded holomorphic semigroup in the sector

$$S^{(p)} = \left\{ z \,\middle|\, |\arg z| < \frac{\pi}{2}\left(1 - \left|\frac{2}{p} - 1\right|\right)\right\}$$

Proof We begin by showing that e^{-tA} is a contraction on all the L^p spaces. First, suppose $f \in L^2$ and $f \ge 0$. Then

$$\|e^{-tA}f\|_1 = (1, e^{-tA}f) = (e^{-tA}1, f) = (1, f) = \|f\|_1$$

If $f \in L^2$ is real-valued, then we write $f = f_+ - f_-$ where $f_+ = \max\{0, f(x)\}$ and $f_- = \max\{0, -f(x)\}$. Then

$$\|e^{-tA}f\|_1 \le \|e^{-tA}f_+\|_1 + \|e^{-tA}f_-\|_1 = \|f_+\|_1 + \|f_-\|_1 = \|f\|_1$$

Finally, suppose $f(x) \in L^2$ is complex-valued. Then

$$\begin{aligned} |(e^{-tA}f)(x)| &= \sup_{\eta \text{ rational}} \{\mathrm{Re}[e^{-i\eta}(e^{-tA}f)(x)]\} \\ &= \sup_{\eta \text{ rational}} \{\mathrm{Re}[(e^{-tA}(e^{-i\eta}f))(x)]\} \\ &= \sup_{\eta \text{ rational}} \{(e^{-tA}(\mathrm{Re}\, e^{-i\eta}f))(x)\} \end{aligned}$$

for almost all x, where we have used the fact that e^{-tA} takes real functions into real functions since e^{-tA} is positivity preserving. Also, for each real $g \in L^2$,

$$\begin{aligned} |(e^{-tA}g)(x)| &= |e^{-tA}g_+ - e^{-tA}g_-| \\ &\le e^{-tA}g_+ + e^{-tA}g_- \\ &= e^{-tA}|g(x)| \end{aligned}$$

almost everywhere. Thus

$$|(e^{-tA}f)(x)| \le e^{-tA}|f(x)| \qquad \text{a.e.} \tag{X.103}$$

which implies that $\|e^{-tA}f\|_1 \le \|e^{-tA}|f(x)|\|_1 = \|f\|_1$. Thus, for all $f \in L^2$, $\|e^{-tA}f\|_1 \le \|f\|_1$.

If $f \in L^\infty \subset L^2$, then

$$\begin{aligned} \|e^{-tA}f\|_\infty &= \sup_{\substack{\|g\|_1 = 1 \\ g \in L^2}} (e^{-tA}f, g) \\ &= \sup_{\substack{\|g\|_1 = 1 \\ g \in L^2}} (f, e^{-tA}g) \\ &\le \|f\|_\infty \left(\sup_{\|g\|_1 = 1} \|e^{-tA}g\|_1 \right) = \|f\|_\infty \end{aligned}$$

so e^{-tA} is a contraction on L^∞ also. Thus by the Riesz–Thorin theorem, e^{-tA} is a contraction on all the L^p spaces. To prove the analyticity statement, we need the Stein interpolation theorem (Theorem IX.21). Because A is positive and self-adjoint, $e^{-\zeta A}$ is analytic for $\mathrm{Re}\,\zeta > 0$, and continuous and bounded by one in the closed right half-plane as an operator on L^2. First, we interpolate between $p = 1$ and $p = 2$. Let $\eta > 0$ and $\theta \in (-\pi/2, \pi/2)$ be fixed. Then for all z satisfying $0 < \mathrm{Re}\, z < 1$, $e^{-\eta e^{i\theta z}A}$ is an analytic operator-valued function on $L^1 \cap L^2 = L^2$. Further, $e^{-\eta e^{i\theta z}A}$ is bounded and continuous on the closed strip $0 \le \mathrm{Re}\, z \le 1$. For $\mathrm{Re}\, z = 1$, $\|e^{-\eta e^{i\theta z}A}f\|_2 \le \|f\|_2$ and for $\mathrm{Re}\, z = 0$, $\|e^{-\eta e^{i\theta z}A}f\|_1 \le \|f\|_1$. Thus, by the Stein interpolation

theorem, for $t \in (0, 1)$, $\|e^{-\eta e^{i\theta_t} A} f\|_p \le \|f\|_p$ where $t = 2 - 2/p$. Since $\eta > 0$ and $\theta \in (-\pi/2, \pi/2)$ were arbitrary, we conclude that

$$\|e^{-\zeta A} f\|_p \le \|f\|_p \qquad \text{whenever} \qquad |\arg \zeta| \le \frac{\pi}{2}\left(2 - \frac{2}{p}\right) = \frac{\pi}{2}\left(1 - \left|\frac{2}{p} - 1\right|\right)$$

The proof for $2 \le p < \infty$ is similar. Now, if f_k and g_k are simple functions, $\int_M (e^{-\zeta A} f_k) g_k \, d\mu$ is analytic in the right half-plane. If $f_k \xrightarrow{L^p} f$ and $g_k \xrightarrow{L^q} g$, where $p^{-1} + q^{-1} = 1$, then

$$\int_M (e^{-\zeta A} f_k) g_k \, d\mu \to \int_M (e^{-\zeta A} f) g \, d\mu$$

uniformly in $S^{(p)} = \{\zeta \mid |\arg \zeta| < (\pi/2)(1 - |(2/p) - 1|)\}$ so $\int_M (e^{-\zeta A} f) g \, d\mu$ is analytic in this sector. Since weakly analytic functions are strongly analytic (Theorem VI.4), $\zeta \to p^{-\zeta A}$ is analytic on $S^{(p)}$ as a function whose values are operators on L^p.

It remains to show that $e^{-zA} f \xrightarrow{L^p} f$ as $z \to 0$ in $S^{(p)}$ for each $f \in L^p$, $1 \le p < \infty$. If $z \in S^{(p)}$ and $1 \le p \le 2$, then $\|e^{-zA} f - f\|_p \le \|e^{-zA} f - f\|_2$ for $f \in L^2$. Since L^2 is dense in L^p, strong continuity follows since $\{e^{-zA}\}$ are uniformly bounded on L^p and e^{-zA} is strongly continuous on L^2. Now, suppose $2 < p < \infty$ and let q satisfy $p^{-1} + q^{-1} = 1$. Suppose that $e^{-t_0 A}\psi = 0$ for some $\psi \in L^q$. Then $e^{-sA}\psi = 0$ for all $s \ge t_0$ and thus by analyticity $e^{-tA}\psi = 0$ for all $t > 0$. Since e^{-tA} is strongly continuous on L^q, $\psi = 0$. Thus $\mathrm{Ker}(e^{-tA}) = \{0\}$ on L^q for each $t > 0$. The reader can easily check that the adjoint of e^{-tA} on L^q is e^{-tA} on L^p. So we conclude that $\mathrm{Ran}(e^{-tA})$ is dense in L^p. Let $\psi = e^{-t_0 A}\varphi$, $\varphi \in L^p$. Then

$$\|e^{-zA}\psi - \psi\|_p \le \|e^{-(z+t_0)A}\varphi - e^{-t_0 A}\varphi\|_p \to 0$$

as $z \to 0$ by the analyticity in the interior of $S^{(p)}$ proved above. Since $\mathrm{Ran}(e^{-t_0 A})$ is dense and the $\{e^{-zA}\}$ are uniformly bounded on $S^{(p)}$, we conclude that e^{-zA} is strongly continuous on L^p. ∎

There are examples where all the hypotheses of Theorem X.55 hold but where e^{-tA} is not strongly continuous on L^∞. In fact, the one-dimensional Hermite operator (Example 1 in Section X.7) provides such an example. For, in that case, $e^{-tA}\psi(x)$ is a continuous function of x for any $t > 0$ if $\psi \in L^\infty$, so $e^{-tA}\psi$ cannot converge in the L^∞-norm to ψ if ψ is not continuous.

X.9 Hypercontractive semigroups

In the previous section we discussed L^p-contractive semigroups. In this section we will prove a self-adjointness theorem for operators of the form $A + V$ where V is a multiplication operator and A generates an L^p-contractive semigroup that satisfies a strong additional property.

Definition Let $\langle M, \mu\rangle$ be a measure space with $\mu(M) = 1$ and suppose that A is a positive self-adjoint operator on $L^2(M, d\mu)$. We say that e^{-tA} is a **hypercontractive semigroup** if:

(i) e^{-tA} is L^p-contractive;
(ii) for some $b > 2$ and some constant C_b, there is a $T > 0$ so that $\|e^{-TA}\varphi\|_b \leq C_b\|\varphi\|_2$ for all $\varphi \in L^2(M, d\mu)$.

By Theorem X.55, condition (i) implies that e^{-tA} is a strongly continuous contraction semigroup for all $p < \infty$. Hölder's inequality shows that

$$\|\cdot\|_q \leq \|\cdot\|_p \quad \text{if} \quad p \geq q \tag{X.104}$$

Thus the L^p-spaces are a nested family of spaces which get smaller as p gets larger; this suggests that (ii) is a very strong condition. The following proposition shows that b plays no special role.

Proposition Let e^{-tA} be a hypercontractive semigroup on $L^2(M, d\mu)$. Then for all $p, q \in (1, \infty)$, there is a constant C_{pq} and a $t_{pq} > 0$ so that if $t \geq t_{pq}$ then

$$\|e^{-tA}\varphi\|_p \leq C_{pq}\|\varphi\|_q$$

for all $\varphi \in L^q$.

Proof The case where $p \leq q$ follows immediately from (i) and (X.104). So suppose that $p > q$. Since $e^{-TA}: L^2 \to L^b$ and $e^{-TA}: L^\infty \to L^\infty$, the Riesz–Thorin theorem implies that there is a constant C so that for all $r \geq 2$, $\|e^{-TA}\varphi\|_r \leq C\|\varphi\|_{br/2}$. We now consider two cases. First, if $q \geq 2$ we choose n large enough so that $2(b/2)^n > p$. Then $\|e^{-nTA}\varphi\|_{(b/2)^n 2} \leq C^n\|\varphi\|_2$, so the conclusion follows if $2 \leq q, p > 2(b/2)^n$, by using (X.104), and hypothesis (i). If $1 < q \leq 2$, then we choose n large enough so that $2(b/2)^n > p$ and $q > c$ where $c^{-1} + (2(b/2)^n)^{-1} = 1$. Since A is self-adjoint and $e^{-nTA}\varphi$ is a bounded map from L^2 to $L^{2(b/2)^n}$, $(e^{-nTA})^* = e^{-nTA}$ is a bounded map from L^c to L^2. Thus e^{-2nTA} is a bounded map from L^c to $L^{2(b/2)^n}$. Since $c < q < p < 2(b/2)^n$, (X.104) implies the proposition. ∎

Before proving the self-adjointness theorem, we present an example of a hypercontractive semigroup.

Example 1 We will use the terminology introduced in Example 2 of Section X.6. Let U: $L^2(\mathbb{R}) \to L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)$ be the unitary map $U: f(x) \to \pi^{1/4}e^{x^2/2}f(x)$, and define $B = UNU^{-1}$. Then

$$B = -\frac{1}{2}\frac{d^2}{dx^2} + x\frac{d}{dx}$$

Since B is unitarily equivalent to N, B is essentially self-adjoint on the set of finite linear combinations of Hermite polynomials, $p_n(x) = U\phi_n$, B is positive, and $Bp_n = np_n$. Thus B generates a contraction semigroup e^{-tB} on $L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)$. We will show that e^{-tB} is a hypercontractive semigroup.

Since $-d/dx^2$, $x^2 - 1$, and $-d^2/dx^2 + (x^2 - 1)$ are all essentially self-adjoint on $\mathscr{S}(\mathbb{R})$, the Trotter product formula (Theorem X.51) implies that

$$e^{-tN}f = \lim_{n\to\infty}\left[\exp\left(\frac{t}{2n}\frac{d^2}{dx^2}\right)\exp\left(-\frac{t}{n}\left(\frac{1}{2}x^2 - 1\right)\right)\right]^n f$$

for all $f \in L^2(\mathbb{R}, dx)$. Since $\exp(-(t/n)(\frac{1}{2}x^2 - 1))$ and $\exp((t/2n)\,d^2/dx^2)$ (Problem 53) are positivity preserving, we conclude that e^{-tN} is positivity preserving. Since U is also positivity preserving, we have shown that e^{-tB} is positivity preserving. Further, $p_0(x) \equiv 1$ and $e^{-tB}p_0 = p_0$. Thus, by Theorem X.55, e^{-tB} is a semigroup of contractions on $L^p(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)$ for each $p \in [1, \infty]$.

To prove hypercontractivity, we will show that $\|e^{-tB}\varphi\|_4 \le C\|\varphi\|_2$ for t large enough. We begin by noticing that

$$\|p_n\|_{L^4(\mathbb{R},\,\pi^{-1/2}e^{-x^2}\,dx)} = \left(\pi^{-1/2}\int_{-\infty}^{\infty}(p_n(x))^4 e^{-x^2}\,dx\right)^{1/4}$$

$$= \|p_n(x)\phi_n\|^{1/2}_{L^2(\mathbb{R},\,dx)}$$

Now, since $A\phi_0 = 0$,

$$\phi_n(x) = (n!)^{-1/2}(A^\dagger)^n\phi_0 = (n!)^{-1/2}2^{n/2}{:}\left(\frac{A + A^\dagger}{\sqrt{2}}\right)^n{:}\phi_0$$

where the Wick power $:((A + A^\dagger)/\sqrt{2})^n:$ is defined by expanding and then moving all the $A^\dagger$ to the left in each term. Since $(A + A^\dagger)/\sqrt{2} = x$, the argument outlined in Problem 48 shows that the operator $:((A + A^\dagger)/\sqrt{2})^n:$

is just multiplication by a polynomial. But $\phi_n(x) = p_n(x)\phi_0$, so for any $\psi \in L^2(\mathbb{R}, dx)$,

$$p_n(x)\psi = 2^{n/2}(n!)^{-1/2} :\left(\frac{A + A^\dagger}{\sqrt{2}}\right)^n : \psi$$

Thus, using the estimate (X.61) we find that

$$\begin{aligned}
\|p_n(x)\phi_n\|_{L^2(\mathbb{R}^n)} &= 2^{n/2}(n!)^{-1/2} \left\| :\left(\frac{A + A^\dagger}{\sqrt{2}}\right)^n : \phi_n \right\|_{L^2(\mathbb{R}^n)} \\
&\leq \frac{2^n}{(n!)^{1/2}} \left((n+1)^{1/2} \cdots (n+n)^{1/2}\right) \\
&= 2^n \left(\frac{(2n)!}{(n!)^2}\right)^{1/2} \\
&\leq 4^n
\end{aligned}$$

Thus, if $\varphi = \sum_{n=0}^\infty a_n p_n(x) \in L^2(\mathbb{R}, \pi^{-1/2} e^{-x^2}\, dx)$, then

$$\begin{aligned}
\left\| e^{-tB} \sum_{n=0}^\infty a_n p_n(x) \right\|_{L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\, dx)} &\leq \sum_{n=0}^\infty |a_n| e^{-tn} \|p_n(x)\|_{L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\, dx)} \\
&\leq \left(\sum_{n=0}^\infty |a_n|^2\right)^{1/2} \left(\sum_{n=0}^\infty e^{-2tn} 4^n\right)^{1/2} \\
&\leq C \|\varphi\|_{L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\, dx)}
\end{aligned}$$

for $t > \frac{1}{2}\log 4$. Therefore e^{-tB} is hypercontractive. We state the result as a theorem:

Theorem X.56 The operator $-\frac{1}{2}\, d^2/dx^2 + x\, d/dx$ on $L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\, dx)$ is positive and essentially self-adjoint on the set of finite linear combinations of Hermite polynomials, and generates a hypercontractive semigroup.

As a preparation for our main theorem, we prove the following result. For generalizations, see the Notes.

Theorem X.57 (Segal's lemma) Let A and B be semibounded self-adjoint operators so that $A + B$ is essentially self-adjoint on $D(A) \cap D(B)$. Then

$$\|e^{-(A+B)}\| \leq \|e^{-A/2} e^{-B} e^{-A/2}\|$$

Proof Let $C = \|e^{-A/2}e^{-B}e^{-A/2}\|$. Let $\varphi \in Q(e^{A})$. Then certainly

$$\varphi \in Q(e^{-B}) = \mathscr{H}$$

and

$$\begin{aligned}(\varphi, e^{-B}\varphi) &= (e^{A/2}\varphi, e^{-A/2}e^{-B}e^{-A/2}e^{A/2}\varphi)\\ &\leq C(\varphi, e^{A}\varphi)\end{aligned}$$

so we conclude that $\|e^{-B/2}\varphi\|^2 \leq C\|e^{A/2}\varphi\|^2$. It follows from Theorem X.18 that $(\varphi, e^{-B/2}\varphi) \leq (\varphi, C^{1/2}e^{-A/2}\varphi)$ or $\|e^{-B/4}\varphi\|^2 \leq C^{1/2}\|e^{A/4}\varphi\|^2$. By induction we have $\|e^{-2^{-n}B}\varphi\|^2 \leq C^{2^{1-n}}\|e^{2^{-n}A}\varphi\|^2$. Thus

$$(\varphi, e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A}\varphi) \leq C^{2^{-n}}(\varphi, \varphi)$$

for all $\varphi \in Q(e^{A})$. Since $e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A}$ is a bounded self-adjoint operator,

$$\|e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A}\| \leq C^{2^{-n}}$$

so

$$\|(e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A})^{2^n}\| \leq C$$

But by the Trotter product formula,

$$(e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A})^{2^n} \xrightarrow[n\to\infty]{} e^{-(A+B)}$$

strongly so $\|e^{-(A+B)}\| \leq C$ also. ∎

We are now ready to state our main theorem.

Theorem X.58 Let $\langle M, \mu\rangle$ be a measure space with $\mu(M) = 1$ and let H_0 be the generator of a hypercontractive semigroup on $L^2(M, d\mu)$. Let V be a real-valued measurable function on $\langle M, \mu\rangle$ such that $V \in L^p(M, d\mu)$ for all $p \in [1, \infty)$ and $e^{-tV} \in L^1(M, d\mu)$ for all $t > 0$. Then $H_0 + V$ is essentially self-adjoint on $C^\infty(H_0) \cap D(V)$ and is bounded below.

Proof The proof of the theorem is fairly long, so we will break it up into several steps. The idea is the following: First define

$$V_n(x) = \begin{cases} V(x) & \text{if } |V(x)| \leq n\\ 0 & \text{otherwise}\end{cases}$$

Then $H_n = H_0 + V_n$ is self-adjoint on $D(H_0)$ by the Kato–Rellich theorem. We will first derive various uniform bounds on e^{-tH_n} as a map from L^p to L^q. We then use these bounds to prove that e^{-tH_n} converges strongly to

a one-parameter self-adjoint semigroup $T(t)$ on $L^2(M, d\mu)$, so that $T(t)$ is generated by a semibounded self-adjoint operator H. Finally, we show that H is essentially self-adjoint on $C^\infty(H_0) \cap D(V)$ and equals $H_0 + V$ there.

Step 1 *For any $t > 0$, $\sup_n \|e^{-tV_n}\|_1 < \infty$ and is uniformly bounded in t in any compact subinterval of $[0, \infty)$.*

To prove this statement, notice that if $V(x) < 0$, then $V_n(x) \geq V(x)$ so $e^{-tV_n(x)} \leq e^{-tV(x)}$. On the other hand, if $V(x) \geq 0$, then $V_n(x) \geq 0$ so that $e^{-tV_n(x)} \leq 1$. Thus, $e^{-tV_n(x)} \leq e^{-tV(x)} + 1$ for all x, so $\|e^{-tV_n(x)}\|_1 \leq \|e^{-tV}\|_1 + 1$. If

$$V_+(x) = \begin{cases} V(x), & V(x) \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

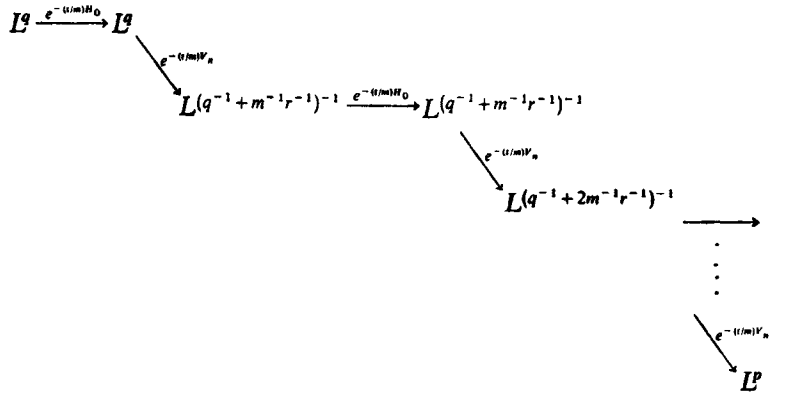
and $V_- = V - V_+$, then $\|e^{-tV_+}\|_1 \leq 1$ and $\|e^{-tV_-}\|_1$ is monotone increasing; the uniformity statement follows easily.

Step 2 *Let $p < q$ be given. Then for each t, there is a constant C_t (depending on q, p, and t but independent of n) so that for all $\varphi \in L^q$,*

$$\|e^{-tH_n}\varphi\|_p \leq C_t\|\varphi\|_q$$

For fixed p and q, C_t is uniformly bounded for t in a compact subinterval of $[0, \infty)$.

Notice that this is a fairly weak result since $p < q$, but the conditions on V are so strong that it will be sufficient when we need it in Step 4. Let $A_m = (e^{-tV_n/m}e^{-tH_0/m})^m$. We will first show that $\|A_m\varphi\|_p \leq C_t\|\varphi\|_q$ and then use the Trotter product formula. Let r satisfy $r^{-1} + q^{-1} = p^{-1}$. Then we can write the map A_m as



Each of the maps $e^{-(t/m)H_0}$ is a contraction since e^{-tH_0} is a hypercontractive semigroup. And by Hölder's inequality, each of the maps $e^{-(t/m)V_n}$ has norm less than or equal to $\|e^{-(t/m)V_n}\|_{mr}$. Thus

$$\|A_m\varphi\|_p \leq \|e^{-(t/m)V_n}\|_{mr}^m \|\varphi\|_q$$

Furthermore,

$$\|e^{-(t/m)V_n}\|_{mr}^m = \left[\left(\int_M e^{-tV_n r}\, d\mu\right)^{1/mr}\right]^m = \|e^{-tV_n}\|_r$$

so we conclude that

$$\|A_m\varphi\|_p \leq \|e^{-tV_n}\|_r \|\varphi\|_q$$

By the Trotter product formula $A_m\varphi \to e^{-tH_n}\varphi$ for all φ in L^2. But, by the weak-* compactness of the unit ball in L^p, $A_m\varphi$ also has a weak-* limit point ψ in L^p with $\|\psi\|_p \leq \|e^{-tV}\|_r\|\varphi\|_q$. A little measure theory now shows that we must have $\psi = e^{-tH_n}\varphi$. This proves the bound. The uniformity follows similarly to the uniformity in Step 1.

Step 3 *There is a constant E, independent of n, so that*

$$\|e^{-tH_n}\varphi\|_2 \leq e^{Et}\|\varphi\|_2$$

We first show that $e^{-TH_0}e^{-2TV_n}e^{-TH_0}$ is a bounded map from L^2 to L^2 with bound D independent of n. Since H_0 is hypercontractive, e^{-TH_0} is a bounded map (with bound D_1) from L^2 to L^4. By Hölder's inequality, e^{-2TV_n} is a bounded map from L^4 to L^2 with bound $\|e^{-2TV_n}\|_4 = \|e^{-8TV_n}\|_1^{1/4} \leq (\|e^{-8TV}\|_1 + 1)^{1/4}$ by Step 1. Finally, e^{-TH_0} is a contraction on L^2 so $\|e^{-TH_0}e^{-2TV_n}e^{-TH_0}\| \leq D$. Thus, by Segal's lemma,

$$\|e^{-2T(H_0+V_n)}\| \leq D$$

or

$$-E \equiv \frac{-\log D}{2T} \leq H_0 + V_n$$

Step 4 *Let $\varphi \in L^2(M, d\mu)$. Then $T(t)\varphi \equiv \lim_{n\to\infty} e^{-tH_n}\varphi$ exists and $T(t)$ is a strongly continuous semigroup of self-adjoint operators satisfying $\|T(t)\| \leq e^{Et}$. Further, there is a unique self-adjoint operator H satisfying $H \geq -E$ so that $T(t) = e^{-tH}$.*

We begin by expressing $e^{-tH_n}\varphi$ for $\varphi \in L^2$ by Duhamel's formula:

$$e^{-tH_n}\varphi = e^{-tH_m}\varphi + \int_0^t e^{-(t-u)H_n}(V_m - V_n)e^{-uH_m}\varphi\, du$$

This formula holds because both sides applied to a vector in $D(H_0)$ solve the same first order differential equation. Since H_n is self-adjoint on $D(H_0)$, the semigroups are equal. Now suppose $\varphi \in L^\infty$ and let t be fixed. Then by Step 2 we can find a constant K_1 so that $\|e^{-uH_m}\varphi\|_8 \leq K_1\|\varphi\|_\infty$ for all m and all $u \in [0, t]$. We can also find K_2 so that

$$\|e^{-(t-u)H_n}\psi\|_2 \leq K_2\|\psi\|_4$$

for all n and all $u \in [0, t]$. Finally, by Hölder's inequality, $V_m - V_n$ has norm $\|V_m - V_n\|_8$ as a map from L^8 to L^4. Thus by Duhamel's formula,

$$\|e^{-tH_n}\varphi - e^{-tH_m}\varphi\|_2 \leq K_1K_2\, t\|V_m - V_n\|_8\|\psi\|_\infty$$

Since $V_n \xrightarrow{L^8} V$, $e^{-tH_m}\varphi$ is Cauchy in L^2; so we can define $T(t)\varphi = \lim_{n\to\infty} e^{-tH_n}\varphi$. By Step 3, $\{e^{-tH_m}\}$ are uniformly bounded for t in compact subintervals of $[0, \infty)$ so an $\varepsilon/3$ argument shows that $e^{-tH_n}\varphi$ converges for all $\varphi \in L^2$. Similarly, since the convergence for $\varphi \in L^\infty$ is uniform on compact t intervals, $T(t)$ is a strongly continuous semigroup. We now define H to be the infinitesimal generator of $T(t)$. Since each e^{-tH} is self-adjoint, H is symmetric. But e^{-tH} is a semigroup bounded by e^{Et} so $-E - 1 \in \rho(H)$. By the fundamental criterion, H is self-adjoint. The bounds follow immediately from Step 3.

Step 5 *Let* $\mathscr{D} = \{\varphi \mid \varphi = e^{-tH}\psi$ *for some* $\psi \in L^\infty\}$. *Then,* $\mathscr{D} \subset L^4 \cap D(H_0)$, H *is essentially self-adjoint on* $\mathscr{D}$, *and if* $\varphi \in \mathscr{D}$, $H\varphi = H_0\varphi + V\varphi$.

L^∞ is dense in L^2, so by the spectral theorem, we know that $\mathscr{D}$ is dense in L^2. Also, by the spectral theorem, it is fairly easy to see that the set $(H + i)[\mathscr{D}]$ is L^2-dense, so H is essentially self-adjoint on $\mathscr{D}$. Now, suppose that $\varphi = e^{-tH}\psi \in \mathscr{D}$. By Step 2, $e^{-tH_n}\psi \in L^4$ and by using Duhamel's formula similarly to the above, one can show that $\{e^{-tH_n}\psi\}_{n=1}^\infty$ is Cauchy in L^4. Since $\varphi_n \equiv e^{-tH_n}\psi \xrightarrow{L^2} \varphi$ we conclude that $\varphi \in L^4 \subset D(V)$. Further, since $V_n \xrightarrow{L^4} V$, we have $V_n\varphi_n \xrightarrow{L^2} V\varphi$.

Now, let $f_n(t) = e^{-tH_n}$ and $f(t) = e^{-tH}$. Then $f_n(t)$ and $f(t)$ are analytic in the open right half-plane and by Step 3, $\|f_n(t)\| \leq e^{E(\mathrm{Re}\, t)}$ uniformly in n. Since $f_n(t) \to f(t)$ on the real axis, we conclude by the Vitali convergence theorem (Problem 33 of Chapter I) that $f_n(t) \to f(t)$ strongly, uniformly on compact subsets of the open right half-plane. It follows by the Cauchy integral theorem that $f_n'(t) \to f'(t)$ strongly, i.e.,

$$H_n\varphi_n \to H\varphi$$

Therefore,

$$H_0\varphi_n = (H_n - V_n)\varphi_n \to (H - V)\varphi$$

Thus, $\varphi \in D(H_0)$ and $H\varphi = H_0\varphi + V\varphi$.

Step 6 $H_0 + V$ *is essentially self-adjoint on* $C^\infty(H_0) \cap D(V)$.

By Step 5, $H_0 + V$ is essentially self-adjoint on $D(H_0) \cap L^4$. Let $\psi \in D(H_0) \cap L^4$ and define $\psi_n = e^{-H_0/n}\psi$. Then by the spectral theorem $\psi_n \in C^\infty(H_0)$ and $H_0\psi_n \to H_0\psi$. But, since e^{-tH_0} is hypercontractive, $\psi_n \in L^4$ and $\psi_n \xrightarrow{L^4} \psi$. Thus, $V\psi_n \xrightarrow{L^2} V\psi$. Therefore

$$D(H_0) \cap L^4 \subset D(\overline{(H_0 + V) \restriction C^\infty(H_0) \cap L^4})$$

Since $L^4 \subset D(V)$, $H_0 + V$ is essentially self-adjoint on $C^\infty(H_0) \cap D(V)$.

This concludes the proof of Theorem X.58. ∎

We remark that if $V \geq 0$, then Step 1 and Step 3 (which uses Theorem X.57) are trivial. We have proven the more difficult theorem since in the main application that we have in mind (Example 4), V is not positive. Theorem X.58 has the following extension:

Theorem X.59 Let $\langle M, \mu\rangle$ be a finite measure space with $\mu(M) = 1$ and let H_0 be the self-adjoint generator of a hypercontractive semigroup on $L^2(M, d\mu)$. Assume that V is a real-valued measurable function on M which satisfies either:

(i) $V \in L^p$ for some $p > 2$ and $\|e^{-tV}\|_1 < \infty$ for all $t \geq 0$

or

(ii) $V \in L^2$ and $V \geq 0$.

Then $H_0 + V$ is essentially self-adjoint on $C^\infty(H_0) \cap D(V)$ and bounded below.

Finally, we state a continuity theorem which can be proven by the methods in the proof of Theorem X.58.

Theorem X.60 Let $\langle M, \mu\rangle$ be a finite measure space with $\mu(M) = 1$ and suppose that the self-adjoint operator H_0 generates a hypercontractive semigroup on $L^2(M, d\mu)$. Let $\{V_n\}_{n=1}^\infty$ and V be real-valued functions on M which satisfy:

(i) $V_n, V \in \bigcap_{p<\infty} L^p(M, d\mu)$

(ii) $e^{-V_n}, e^{-V} \in \bigcap_{p<\infty} L^p(M, d\mu)$

(iii) There is a $q \in (2, \infty]$ so that

$$V_n \xrightarrow{L^q} V \qquad \text{and} \qquad \sup_n \|e^{-V_n}\|_q < \infty$$

Then $H_0 + V_n \to H_0 + V$ in norm-resolvent sense.

Example 2 (the anharmonic oscillator, fourth proof) Let $V(x)$ be a non-negative measurable function on $\mathbb{R}$ which satisfies $\int_{-\infty}^{\infty} |V(x)|^p e^{-x^2}\, dx < \infty$ for all $p \in [1, \infty)$. Consider the operator $-d^2/dx^2 + 2x\, d/dx + (V(x) - 1)$ on the set $U[\mathscr{S}]$ where $U: L^2(\mathbb{R}) \to L^2(\mathbb{R}, \pi^{-1/2} e^{-x^2}\, dx)$ is the map defined in Example 1. In Example 1 we showed that $-d^2/dx^2 + 2x\, d/dx$ generates a hypercontractive semigroup. Thus, since $V(x) - 1$ satisfies the conditions of Theorem X.58, $-d^2/dx^2 + 2x\, d/dx + V(x) - 1$ is essentially self-adjoint on $U[\mathscr{S}]$. Therefore $-d^2/dx^2 + x^2 + V(x)$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$. In particular, if we take $V(x) = x^4$, we have another proof of the essential self-adjointness of the anharmonic oscillator on $\mathscr{S}(\mathbb{R})$.

Example 3 Let $V \in L^2(\mathbb{R}^n, \pi^{-n/2} e^{-|x|^2}\, d^n x)$ and $V \geq 0$. Theorem X.59 provides a proof that $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ as follows: By generalizing Example 1, one shows that $-\Delta + 2x \cdot \nabla$ generates a hypercontractive semigroup on $L^2(\mathbb{R}^n, \pi^{-n/2} e^{-|x|^2}\, d^n x)$ so by Theorem X.59 and the method of Example 2, $-\Delta + x^2 + V$ is essentially self-adjoint on $C^\infty(-\Delta + x^2) \cap D(V) = \mathscr{S}(\mathbb{R}^n) \cap D(V)$. By a simple argument, it is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. Finally, as in Example 6 of Section X.2, one uses

$$[x_i, [x_j, -\Delta]] = \delta_{ij}$$

to prove that

$$\|x^2 \psi\|^2 \leq \|(-\Delta + V + x^2)\psi\|^2 + 2n\|\psi\|^2$$

so by Konrady's trick, $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. We have already proven this result in Section X.4 by using Kato's inequality.

Example 4 (application to quantum field theory) We will use the notation introduced in Section X.7.

Theorem X.61 Let $\mathscr{H}$ be a separable Hilbert space with complex conjugation C. Let A be a self-adjoint operator on $\mathscr{H}$ which commutes with C. Then

(a) If $A \geq 0$, then $\Gamma(e^{-tA})$ is an L^p-contractive semigroup on Q-space.
(b) If $A \geq cI > 0$, then $\Gamma(e^{-tA})$ is a hypercontractive semigroup.

Proof We will prove (a). The proof of (b) is essentially an infinite-dimensional version of the corresponding proof in Example 1 (see the Notes

for a reference). Let A_n be a sequence of bounded self-adjoint operators whose spectra consist of finitely many eigenvalues of finite multiplicity so that $e^{-tA_n} \to e^{-tA}$ strongly as $n \to \infty$. Fix n, and let $\{a_\ell\}_{\ell=1}^N$ denote the non-zero eigenvalues of A_n with corresponding eigenfunctions $\{\psi_\ell\}_{\ell=1}^N$. Let $\{\psi_\ell\}_{\ell=N+1}^\infty$ be an orthonormal basis for the kernel of A_n. Let S be the unitary map of $\mathscr{F}_s(\mathscr{H})$ onto the Q space $L^2(Q, d\mu)$ constructed by using the basis $\{\psi_\ell\}_{\ell=1}^\infty$ for $\mathscr{H}$. We will show that SA_nS^{-1} is positivity preserving. If $\varphi(\cdot)$ and $\pi(\cdot)$ are the canonical field and conjugate momentum corresponding to C, then on the subspace $\{P(\varphi(\psi_\ell))\Omega_0 \mid P \text{ a polynomial}\}$ of $\mathscr{F}_s(\mathscr{H})$ the operator $d\Gamma(A_n)$ equals $\frac{1}{2}(\varphi(\psi_\ell)^2 + \pi(\psi_\ell)^2 - 1)$. Thus

$$Sd\Gamma(A_n)S^{-1} = \sum_{\ell=1}^{N} \frac{1}{2} a_\ell \left(-\frac{d^2}{dq_\ell^2} + 2q_\ell \frac{d}{dq_\ell} \right)$$

Therefore,

$$S\Gamma(e^{-tA_n})S^{-1} = \prod_{\ell=1}^{N} \exp\left(-\frac{ta_\ell}{2} \left(-\frac{d^2}{dq_\ell^2} + 2q_\ell \frac{d}{dq_\ell} \right) \right)$$

By Example 1, each $\exp(-(ta_\ell/2)(-d^2/dq_\ell^2 + 2q_\ell\, d/dq_\ell))$ is positivity preserving and

$$\exp\left(-\frac{ta_\ell}{2} \left(-\frac{d^2}{dq_\ell^2} + 2q_\ell \frac{d}{dq_\ell} \right) \right) 1 = 1$$

Thus, $S\Gamma(e^{-tA_n})S^{-1}$ is positivity preserving and $S\Gamma(e^{-tA_n})S^{-1}1 = 1$. Since e^{-tA_n} converges strongly to e^{-tA} on $\mathscr{H}$, $\Gamma(e^{-tA_n})$ converges strongly to $\Gamma(e^{-tA})$ on $\mathscr{F}_s(\mathscr{H})$. We conclude that $S\Gamma(e^{-tA})S^{-1}$ is positivity preserving and satisfies $S\Gamma(e^{-tA})S^{-1}1 = 1$. Therefore, by Theorem X.55, $S\Gamma(e^{-tA})S^{-1}$ is L^p-contractive. ∎

Corollary The free Hamiltonian $d\Gamma(\mu)$ of the free scalar field theory of mass $m > 0$ generates a hypercontractive semigroup $\Gamma(e^{-t\mu})$ on $\mathscr{F}_s(\mathscr{H})$.

Theorem X.62 The spatially cut-off Hamiltonian $H_0 + H_I(g)$ (defined in Section X.7) for a $(\varphi^4)_2$ self-interacting scalar field theory is essentially self-adjoint on $C^\infty(H_0) \cap D(H_I(g))$.

Proof Theorem X.45 and the above corollary show that SH_0S^{-1} and $SH_I(g)S^{-1}$ satisfy the hypotheses of Theorem X.58. ∎

X.10 Graph limits

In this section we continue the discussion of graph limits begun in Section VIII.7, using without comment the notation introduced there. In Theorem VIII.26 we showed that if $\{A_n\}_{n=1}^{\infty}$ *and* A are self-adjoint operators then $A_n \to A$ in the strong resolvent sense if and only if A is the strong graph limit of $\{A_n\}_{n=1}^{\infty}$. Although Theorem VIII.26 is interesting, it is not too useful since the proof depends heavily on the assumed existence of the self-adjoint limit A. In applications, it is often the self-adjointness of this limit which one is trying to establish. If we only assume that $(A_n + i)^{-1}$ and $(A_n - i)^{-1}$ converge strongly to operators R_+ and R_-, then the strong resolvent limit A exists if and only if either R_+ or R_- has dense range (Theorem VIII.22), a property which can be difficult to prove. On the other hand, the strong graph limit of a sequence of self-adjoint operators $\{A_n\}$ may exist but may not be self-adjoint, though it is automatically closed and symmetric (Theorem VIII.27). The point of the following theorem is that if *both* types of limit exist, then the limiting operator is self-adjoint. In fact, one need only use weak graph limits.

Theorem X.63 (graph limit theorem) Let $\{A_n\}_{n=1}^{\infty}$ be a sequence of self-adjoint operators on a Hilbert space $\mathscr{H}$. Suppose that:

(i) $(A_n \pm i)^{-1} \to R_{\pm}$ strongly

and

(ii) The weak graph limit A of $\{A_n\}_{n=1}^{\infty}$ is densely defined.

Then A is self-adjoint, $(A \pm i)^{-1} = R_{\pm}$, and A_n converges to A in strong resolvent sense.

Proof We first show that $\mathrm{Ker}(R_+) = \{0\}$. Let $\chi \in \mathrm{Ker}(R_+)$ and $\varphi \in D(A)$. Then there exists $\{\varphi_n\}_{n=1}^{\infty}$ with $\varphi_n \in D(A_n)$, $\varphi_n \to \varphi$, and $A_n\varphi_n \xrightarrow{w} A\varphi$. Thus

$$\begin{aligned}(\chi, \varphi) &= \lim_{n\to\infty} (\chi, \varphi_n) \\ &= \lim_{n\to\infty} ((A_n + i)^{-1}\chi, (A_n - i)\varphi_n) \\ &= (R_+\chi, A\varphi - i\varphi) \\ &= 0\end{aligned}$$

Since $D(A)$ is dense, $\chi = 0$. Thus $\mathrm{Ker}(R_+) = \{0\}$. Since $R_- = R_+^*$, $\mathrm{Ran}\, R_- = (\mathrm{Ker}\, R_+)^{\perp} = \mathscr{H}$. Therefore, by Theorem VIII.22, there is a self-adjoint

operator A' so that $A_n \to A'$ in strong resolvent sense. Finally, Theorem VIII.26 implies that A' is the strong graph limit of $\{A_n\}$ so $A' \subset A$. But by Theorem VIII.28, A is symmetric, so $A' = A$. ∎

This theorem is important because it reduces the self-adjointness question to convergence questions, and these problems can sometimes be handled directly by estimates on the operators A_n. We will illustrate this with condition (i) first. Later we give a sufficient condition for (ii). How can one prove (i)? If $\varphi \in \mathscr{H}$, then *formally*

$$(A_n + i)^{-1}\varphi - (A_m + i)^{-1}\varphi = (A_n + i)^{-1}(A_n - A_m)(A_m + i)^{-1}\varphi \tag{X.105}$$

This expression makes sense if $(A_m + i)^{-1}\varphi$ is both in $D(A_n)$ and $D(A_m)$. Thus, if m and n are fixed and we want (X.105) to hold for a dense set, we must require that $D_{n,m} \equiv (A_m + i)[D(A_n) \cap D(A_m)]$ be dense. Further if we want to take the limit of (X.105) for a fixed φ, we must require $\varphi \in \bigcap D_{n,m}$. Thus we cannot hope to use (X.105) unless $\bigcap D_{n,m}$ is dense. Once we have this regularity condition, then we can prove that the resolvents converge if both $A_n - A_m$ and $(A_m \pm i)^{-1}$ can be estimated uniformly in terms of an auxiliary self-adjoint operator:

Theorem X.64 Let $\{A_n\}$ be a sequence of self-adjoint operators with a common core D_0. Let N be a strictly positive self-adjoint operator so that for some $\alpha > 0$, $\beta > 0$:

(i) $\mathscr{D}^{\pm} = \bigcap_n (\mathrm{Ran}(A_n \pm i) \restriction D_0)$ are dense and $\mathscr{D}^{\pm} \subset D(N^{\alpha})$.
(ii) $\|N^{\beta}(A_n \pm i)^{-1}N^{-\alpha}\| \leq M$ for all n.
(iii) N^{β} is essentially self-adjoint on D_0 and

$$\|N^{-\beta}(A_n - A_m)N^{-\beta}\| \to 0 \qquad \text{as} \quad n, m \to \infty$$

Then, for each $\varphi \in \mathscr{H}$, $\{(A_n \pm i)^{-1}\varphi\}$ is a Cauchy sequence in $\mathscr{H}$.

Proof Let $\chi \in \mathscr{D}^{+}$ and define $\varphi_n = (A_n + i)^{-1}\chi$. Then

$$\begin{aligned}
\|\varphi_n - \varphi_m\|^2 &= (\varphi_n - \varphi_m, \varphi_n - \varphi_m) \\
&= \mathrm{Im}(\varphi_n - \varphi_m, (A_n + i)(\varphi_n - \varphi_m)) \\
&\leq |(\varphi_n - \varphi_m, (A_n + i)(\varphi_n - \varphi_m))| \\
&= |(\varphi_n - \varphi_m, (A_m - A_n)\varphi_m)| \\
&= |(N^{\beta}(\varphi_n - \varphi_m), N^{-\beta}(A_m - A_n)N^{-\beta}N^{\beta}\varphi_m)| \\
&\leq (2 \sup_k \|N^{\beta}(A_k + i)^{-1}N^{-\alpha}N^{\alpha}\chi\|^2)\|N^{-\beta}(A_m - A_n)N^{-\beta}\| \\
&\leq 2M^2\|N^{\alpha}\chi\|^2\|N^{-\beta}(A_m - A_n)N^{-\beta}\| \\
&\to 0 \qquad \text{as} \quad n, m \to \infty
\end{aligned}$$

Thus, $(A_n + i)^{-1}$ is strongly Cauchy on $\mathscr{D}^+$. Since $\mathscr{D}^+$ is dense and the $(A_n + i)^{-1}$ are uniformly bounded, $(A_n + i)^{-1}\varphi$ converges for all $\varphi \in \mathscr{H}$. The proof for $(A_n - i)^{-1}$ is the same. ∎

Example (the anharmonic oscillator, fifth proof) Let

$$H_0 = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right)$$

on $\mathscr{H} = L^2(\mathbb{R})$ and $V = x^4$. In the notation of Example 2 of Section X.6, $H_0 = A^\dagger A + \frac{1}{2}$ and $V = \frac{1}{4}(A + A^\dagger)^4$. Let E_n be the spectral projection of H_0 corresponding to the interval $[0, n]$. The range of E_n is finite dimensional and consists of the first n Hermite functions. We take D_0 to be the set of finite linear combinations of Hermite functions, set $A_n = H_0 + V_n$ where $V_n = E_n V E_n$, and $N = H_0$. We will show that A_n, N, and D_0 satisfy the hypotheses of Theorem X.64 with $\beta = 2$ and $\alpha = 1$. D_0 is a core for H_0, so since each $E_n V E_n$ is bounded, D_0 is a common core for $\{A_n\}_{n=1}^{\infty}$. To prove (i) notice that $\mathrm{Ran}[(A_n \pm i) \restriction (E_n\mathscr{H})] = E_n\mathscr{H}$ since A_n leaves $E_n\mathscr{H}$ invariant, $A_n \restriction E_n\mathscr{H}$ is self-adjoint, and $E_n\mathscr{H}$ is finite dimensional. On the other hand, the spectral theorem shows that $\mathrm{Ran}[(A_n \pm i) \restriction (D_0 \cap (I - E_n)\mathscr{H})] = D_0 \cap (I - E_n)\mathscr{H}$ since $A_n = H_0$ on $(I - E_n)\mathscr{H}$. Thus $\mathrm{Ran}(A_n \pm i) \restriction D_0 \supset D_0$. The converse inclusion holds trivially so we have $\mathscr{D}^{\pm} = \bigcap_n \mathrm{Ran}(A_n + i) \restriction D_0 = D_0$. Further, by the spectral theorem all powers of $N = H_0$ are essentially self-adjoint on D_0. The estimate in (iii) follows immediately from the fact that $V = \frac{1}{4}(A^\dagger + A)^4$ and the estimates (X.61). It remains to prove the estimate in (ii), i.e., that for $\varphi \in D_0$,

$$\|N^2(A_n \pm i)^{-1}N^{-1}\varphi\| \leq M\|\varphi\| \tag{X.106}$$

This is equivalent to showing that

$$N^4 \leq M_1(A_n \mp i)N^2(A_n \pm i) + M_2 \tag{X.107}$$

as quadratic forms on D_0. To prove (X.107) we expand:

$$\begin{aligned}(A_n \mp i)N^2(A_n \pm i) &= (N + V_n \mp i)N^2(N + V_n \pm i)\\ &= N^4 + V_n N^3 + N^3 V_n + (V_n \mp i)N^2(V_n \pm i)\\ &= N^4 + N^{3/2}V_n N^{3/2} + [N^{3/2}, [N^{3/2}, V_n]]\\ &\quad + (V_n \mp i)N^2(V_n \pm i)\\ &\geq N^4 + [N^{3/2}, [N^{3/2}, V_n]]\end{aligned} \tag{X.108}$$

since V_n and N are positive operators. Using the estimate (X.61) and the commutation properties of $A^\dagger$ and A, one can prove (Problem 62) that for any $\varepsilon > 0$, there is a b so that

$$\|[N^{3/2}, [N^{3/2}, V_n]]\varphi\| \leq \varepsilon\|N^4\varphi\| + b\|\varphi\|$$

for all $\varphi \in D_0$ and all n. Choosing ε small enough so that $2\varepsilon < 1$ we can conclude by Theorem X.18 that

$$[N^{3/2}, [N^{3/2}, V_n]] \leq 2\varepsilon N^4 + M_2 \tag{X.109}$$

as quadratic forms on D_0. Combining (X.108) and (X.109) we have (X.107), which proves the estimate in (ii).

We have thus verified that the hypotheses of Theorem X.64 hold for the sequence $H_0 + V_n$. Therefore, $(H + V_n \pm i)^{-1}$ converge strongly on $\mathscr{H}$. Furthermore, to apply Theorem X.63 we only need to show that $D^s_\infty = \{\psi \mid \langle\psi, \varphi\rangle \in \Gamma^s_\infty \text{ for some } \varphi\}$ is dense. In our case this is trivial since for all $\psi \in D_0$ we have $(H_0 + V_n)E_n\psi \to H_0\psi + x^4\psi$. Therefore by Theorem X.63, $H_0 + V_n$ converges in the strong resolvent sense to a self-adjoint operator C whose domain contains D_0 and $C \restriction D_0 = \frac{1}{2}(-d^2/dx^2 + x^2) + x^4$.

This existence result is not particularly interesting since we could have immediately concluded from Theorem X.3 that $\frac{1}{2}(-d^2/dx^2 + x^2 + 2x^4) \restriction D_0$ has a self-adjoint extension. But, the following argument using the resolvent convergence allows us to prove self-adjointness on $D(H_0) \cap D(x^4)$. First we expand $(H_0 + V_n)^2$ finding that (as quadratic forms on D_0)

$$\begin{aligned}(H_0 + V_n)^2 &= H_0^2 + V_n^2 + H_0 V_n + V_n H_0 \\ &= H_0^2 + V_n^2 + 2H_0^{1/2} V_n H_0^{1/2} + [H_0^{1/2}, [H_0^{1/2}, V_n]] \\ &\geq H_0^2 + V_n^2 + [H_0^{1/2}, [H_0^{1/2}, V_n]]\end{aligned}$$

since $V_n \geq 0$. A similar technique to the one outlined in Problem 62 to prove (X.109) can be used to prove that for any $\varepsilon > 0$ there is a constant b (independent of n) so that

$$0 \leq \varepsilon H_0^2 + [H_0^{1/2}, [H_0^{1/2}, V_n]] + b \tag{X.110}$$

Thus, there are constants c_1 and c_2 so that for $\varphi \in D_0$ and all n,

$$\|H_0\varphi\|^2 + \|V_n\varphi\|^2 \leq c_1\|(H_0 + V_n)\varphi\|^2 + c_2\|\varphi\|^2 \tag{X.111}$$

Now, let $\psi \in D(C)$. Then $\psi = (C + i)^{-1}\chi$ for some χ in $\mathscr{H}$. If we set $\psi_n = (H_0 + V_n + i)^{-1}\chi$, then $\psi_n \to \psi$. Thus, for each $\theta \in D_0$,

$$|(V\theta, \psi)| \leq \|V\theta\|\,\|\psi - \psi_n\| + \|(V - V_n)\theta\|\,\|\psi_n\| + |(\theta, V_n\psi_n)| \tag{X.112}$$

But from (X.111) it follows that

$$\begin{aligned}\|V_n\psi_n\| &\leq d_1\|(H_0 + V_n)\psi_n\| + d_2\|\psi_n\| \\ &\leq (d_1 + d_2)\|(H_0 + V_n + i)\psi_n\| = (d_1 + d_2)\|\chi\|\end{aligned}$$

Since the first two terms in (X.112) go to zero as $n \to \infty$, we conclude that $|(V\theta, \psi)| \leq (d_1 + d_2)\|\theta\|\ \|\chi\|$ for all $\theta \in D_0$. Thus $\psi \in D((V \restriction D_0)^*) = D(V)$, so $D(C) \subset D(V)$. A similar proof shows that $D(C) \subset D(H_0)$. Therefore, $C = \frac{1}{2}(-d^2/dx^2 + x^2) + x^4$ is self-adjoint on $D(-d^2/dx^2 + x^2) \cap D(x^4)$.

This example gives the main ideas of the first self-adjointness proof for the spatially cut-off $(\varphi^4)_2$ Hamiltonian in quantum field theory. In the field theory case, the proofs of the estimates (X.109) and (X.110) are more difficult but use many of the same ideas (Problem 62).

We turn now to the problem of proving the condition (ii) of Theorem X.63. Since (ii) is sometimes difficult to verify directly, it is useful to have the following consequence of Theorem X.63. First, we make a definition.

Definition A sequence $\{A_n\}_{n=1}^{\infty}$ of positive self-adjoint operators is called **densely bounded** if there is a dense set $D_b \subset \mathscr{H}$ so that for any $\psi \in D_b$, there is a sequence $\{\psi_n\}_{n=1}^{\infty}$ so that

(i) $\psi_n \xrightarrow{\mathscr{H}} \psi$
(ii) $\psi_n \in Q(A_n)$
(iii) $\sup_n (\psi_n, A_n\psi_n) < \infty$

Theorem X.65 Let A_n be a sequence of positive self-adjoint operators on a Hilbert space $\mathscr{H}$. Suppose:

(i) $(A_n + 1)^{-1}$ converges to R strongly.
(ii) $\{A_n\}_{n=1}^{\infty}$ is densely bounded.

Then there is a self-adjoint operator A with $R = (A + 1)^{-1}$ so that $A_n \to A$ in strong resolvent sense.

Proof Let $B_n = (A_n + 1)^{1/2}$. Then $B_n^{-2} \to R$ strongly and since the B_n^{-2} are uniformly bounded positive operators, the continuity of the functional calculus for the square root (Theorem VIII.20 or Problem VI.14) implies that $B_n^{-1} \to R^{1/2}$ strongly. If we can show that there is a subsequence $\{B_{n_k}\}$ of $\{B_n\}$ so that the weak graph limit of $\{B_{n_k}\}$ is densely defined, then by a slight modification of Theorem X.63, we can conclude that $R^{1/2} = B^{-1}$ for some positive self-adjoint B. If we then set $A = B^2 - 1$, we have $R = (A + 1)^{-1}$ which proves the theorem.

We construct the subsequence of $\{B_n\}$ as follows. Let $\{\psi^{(k)}\}_{k=1}^{\infty}$ be a total set of vectors in D_b. Since $\{A_n\}_{n=1}^{\infty}$ is densely bounded, for each k we can find a sequence $\{\psi_n^{(k)}\}_{n=1}^{\infty}$ so that $\psi_n^{(k)} \in Q(A_n) = D(B_n)$, $\psi_n^{(k)} \to \psi^{(k)}$, and $\sup_n \|B_n \psi_n^{(k)}\| < \infty$. Now, consider the sequence $B_n \psi_n^{(1)}$. Since all the $B_n \psi_n^{(1)}$ are contained in a fixed ball in $\mathscr{H}$, we can find a weakly convergent subsequence $B_{n(1,j)} \psi_{n(1,j)}^{(1)}$ (because the balls are weakly sequentially compact). Similarly we choose a sequence $\psi_{n(1,j)}^{(2)} \to \psi^{(2)}$ and extract a subsequence of $B_{n(1,j)}$, call it $B_{n(2,j)}$, so that $B_{n(2,j)} \psi_{n(2,j)}^{(2)}$ is weakly convergent. We continue in this way and then (using the diagonalization trick) extract the subsequence $\{B_{n(j,j)}\}_{j=1}^{\infty}$ which has the property that for each k, there is a sequence $\psi_{n(j,j)}^{(k)}$ so that $\psi_{n(j,j)}^{(k)} \in D(B_{n(j,j)})$, $\psi_{n(j,j)}^{(k)} \to \psi^{(k)}$, and $B_{n(j,j)} \psi_{n(j,j)}^{k}$ converges weakly. Thus each $\psi^{(k)}$ is in D_∞^w for the sequence $B_{n(j,j)}$. Since D_b is dense and $\{\psi^{(k)}\}_{k=1}^{\infty}$ is total in D_b, D_∞^w is dense, which shows (by Theorem XIII.28) that the weak graph limit of the sequence $\{B_{n(j,j)}\}_{j=1}^{\infty}$ exists. ∎

This theorem has been applied to prove the existence of the spatially cut-off Hamiltonian in the Yukawa field theory in two dimensions. The details of the proof require the development of the free fermion field and several different sets of difficult estimates. Given the estimates, the idea is as follows: First, the interaction Hamiltonian $H(g, \kappa) = H_0 + H_I(g, \kappa)$ with both spatial and ultraviolet cut-offs is introduced. The spatial cut-off is similar to the spatial cut-off for the $(\varphi^4)_2$ field theory introduced in Section X.7. The ultraviolet cut-off means that the momentum space integral expressing H_I in terms of creation and annihilation operators is restricted to the region $|k| \leq \kappa$. Although $H(g, \kappa)$ makes sense on Fock space, $H(g, \kappa)$ "diverges" as $\kappa \to \infty$. A formal perturbation theory argument suggests that $H(g, \kappa)$ *should* diverge (!) because we have introduced the free field theory mass as an input parameter instead of the physically measurable interacting mass m and further because the free ground state should differ from the interacting ground state by an infinite amount of energy. The perturbation theory argument suggests that the "correct" Hamiltonian should be

$$H = H_0 + H_I - M - E \tag{X.113}$$

where E is given by a divergent integral and M is a well-defined operator multiplied by another divergent integral. Although H_I, M, and E are infinite on Fock space, H should be well defined because of cancellations. If we introduce spatial and momentum cut-off as described above, then

H_0, $H_I(g, \kappa)$, $M(g, \kappa)$, and $E(\kappa)$ are all finite and well defined on Fock space and

$$H_{\text{ren}}(g, \kappa) \equiv H_0 + H_I(g, \kappa) - M(g, \kappa) - E(\kappa)$$

is self-adjoint for each κ. Furthermore, it can be proven that $H_{\text{ren}}(g, \kappa)$ is bounded below uniformly in κ (say by C), that $(H_{\text{ren}}(g, \kappa) - C + 1)^{-1}$ converges strongly, and that $\{H_{\text{ren}}(g, \kappa)\}_{n=1}^{\infty}$ is densely bounded. Thus by Theorem X.65, $H_{\text{ren}}(g, \kappa)$ converges in norm resolvent sense to a self-adjoint operator $H(g)$. $H(g)$ is the "correct" spatially cut-off Hamiltonian. The spatial cut-off must be removed by other methods (see Chapter XIX).

X.11 The Feynman–Kac formula

Let H_0 be the free quantum mechanical Hamiltonian $-\Delta$ and let V be a potential so that $-\Delta + V$ is essentially self-adjoint on $D(-\Delta) \cap D(V)$. Then the Trotter product formula tells us how to express $e^{-it(H_0+V)}$ as a limit of products of $e^{-(it/n)H_0}$ and $e^{-(it/n)V}$ as $n \to \infty$. Since we have an explicit expression for e^{itH_0} as an integral operator (see (IX.31)),

$$(e^{-itH_0}f)(x) = \text{l.i.m.}(4\pi it)^{-3/2} \int_{\mathbb{R}^3} \exp\left(\frac{i|x-y|^2}{4t}\right) f(y)\, dy \qquad \text{(X.114)}$$

we can express $e^{-it(H_0+V)}$ as a limit of integral operators.

Theorem X.66 Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Then

$$(e^{-it(H_0+V)}f)(x_0) = \lim_{n\to\infty} \left(\frac{4\pi it}{n}\right)^{-3n/2} \int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3} \exp(iS_n(x_0, \ldots, x_n, t)) \times f(x_n)\, dx_n \cdots dx_1 \qquad \text{(X.115)}$$

where

$$S_n(x_0, x_1, \ldots, x_n, t) = \sum_{i=1}^{n} \frac{t}{n} \left[\frac{1}{4}\left(\frac{|x_i - x_{i-1}|}{t/n}\right)^2 - V(x_i)\right]$$

(All integrals taken in the sense $\int_{\mathbb{R}^3} = \lim_{m\to\infty} \int_{|x|\le m}$ and all limits taken in the L^2 sense.)

Proof Since $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, $H_0 + V$ is self-adjoint on $D(H_0)$ (Theorem X.15) and thus the Trotter product formula (Theorem VIII.30)

$$e^{-it(H_0+V)}f = \lim_{n\to\infty} (e^{-(it/n)H_0}e^{-(it/n)V})^n f$$

is applicable. The theorem follows by substituting the explicit expressions for $e^{-i(t/n)H_0}$ and $e^{-i(t/n)V}$. ∎

Formula (X.115) was stated by Feynman in 1948 on the basis of a physical interpretation. If a classical particle of mass m moves in a potential V, the smooth path $\omega(s)$, $0 \le s \le t$, is said to have **action** equal to

$$S(\omega) = \int_0^t \left(\frac{m}{2} |\dot{\omega}(s)|^2 - V(\omega(s)) \right) ds \tag{X.116}$$

The principle of least action of Lagrange says that the classical particle will travel the path of least action; i.e., the classical path will satisfy the Euler–Lagrange equation

$$m\ddot{\omega}(t) = -\nabla V(\omega(t))$$

corresponding to (X.116).

To see how to interpret (X.115) in terms of the action, take $m = \frac{1}{2}$ so that $H_0 = -(2m)^{-1}\Delta = -\Delta$. Given $x_0, x_1, \ldots, x_n$, consider a classical particle of mass $\frac{1}{2}$ moving along the polygonal path in Figure X.7 with constant velocity along each segment. The classical action of this path is

$$S(\omega) = \sum_{i=1}^{n} \left(\frac{t}{n}\right) \frac{1}{4} \left(\frac{|x_i - x_{i-1}|}{t/n} \right)^2 - \int_0^t V(\omega(t))\, dt$$

which approximately equals

$$S_n(x_0, x_1, \ldots, x_n, t) = \sum_{i=1}^{n} \left(\frac{t}{n}\right) \left[\frac{1}{4} \left(\frac{|x_i - x_{i-1}|}{t/n} \right)^2 - V(x_i) \right]$$

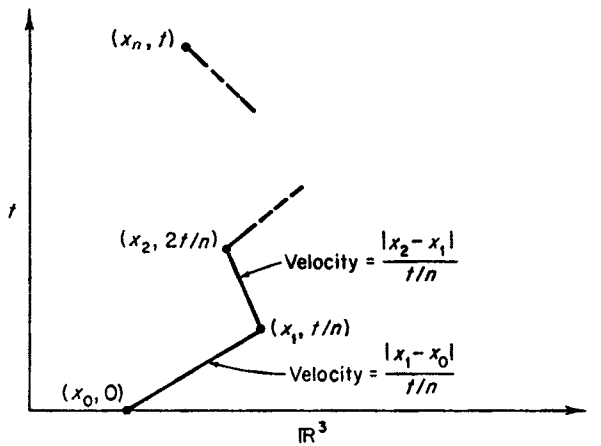


FIGURE X.7 A polygonal path between x_0 and x_n.

if V is continuous and the points $x_0, \ldots, x_n$ are close enough together. Thus

$$(4\pi it/n)^{-3n/2} \int \cdots \int e^{iS_n(x_0, \ldots, x_n, t)} f(x_n)\, dx_n\, dx_{n-1} \cdots dx_1$$

can be interpreted as an integral over all polygonal paths where S_n approximates the action of a classical particle moving along the path as indicated in Figure X.7. As $n \to \infty$, the set of polygonal paths becomes intuitively the set of all paths and given a path ω, $S_n(x_0, \ldots, x_n, t)$ approaches $S(\omega)$ if $\omega(0) = x_0$, $\omega(t) = x_n$, and the x_i lie on ω. Thus, intuitively, one can hope to find a formula for $(e^{-it(H_0+V)}f)(x_0)$ of the form

$$(e^{-it(H_0+V)}f)(x_0) = \int_{\Omega_{x_0}} e^{iS(\omega)} f(\omega(t))\, d\omega \tag{X.117}$$

where Ω_{x_0} is the set of all paths with $\omega(0) = x_0$, $S(\omega)$ is the classical action of the path ω, and $d\omega$ is a measure on Ω_{x_0}. In a natural way, the classical limit can be realized using this formula. If we put Planck's constant back in the Hamiltonian, then the formula reads

$$(e^{-it/\hbar(H_0+V)}f)(x_0) = \int_{\Omega_{x_0}} e^{iS(\omega)/\hbar} f(\omega(t))\, d\omega \tag{X.118}$$

As we take the classical limit by letting $\hbar$ go to zero, the oscillating phases in $e^{iS(\omega)/\hbar}$ tend to cancel except around paths where $S(\omega)$ is stationary. That is, most of the contribution to the dynamics comes from paths nearer and nearer to the classical paths as $\hbar \to 0$.

The above discussion shows why (X.117) is a beautiful heuristic formula. There is a mathematical notion of integration over paths introduced by Wiener, but unfortunately this notion *cannot* be used to make sense out of the right-hand side of (X.118). However, it can be used to derive an analogous formula for $(e^{-t(H_0+V)}f)(x_0)$ called the Feynman–Kac formula. Before proving this formula, we first need to discuss Wiener measure. Our construction of Wiener measure (using only our bare hands) is the most direct. We emphasize that there is an alternative approach using Gaussian random variables and the theory of Markov processes. This more natural approach provides an intuition which is invaluable for further developments, but introducing the necessary probabilistic machinery would take us too far afield. However, we feel that a discussion of the existence of dynamics would be incomplete without presenting the Feynman–Kac formula.

To motivate out construction of Wiener measure on $\mathbb{R}^n$ notice that the Trotter product formula implies that for suitable V,

$$e^{-t(H_0+V)}f = \lim_{m \to \infty} (e^{-(t/m)H_0} e^{-(t/m)V})^m f$$

with

$$(e^{-(t/m)H_0}e^{-(t/m)V})^m f = \int \cdots \int p\left(x_0, x_1; \frac{t}{m}\right) e^{-(t/m)V(x_1)} \cdots$$

$$\times\, p\left(x_{m-1}, x_m; \frac{t}{m}\right) e^{-(t/m)V(x_m)} f(x_m)\, dx_1 \cdots dx_m \quad \text{(X.119)}$$

where

$$p(x, y; t) = (4\pi t)^{-n/2} e^{-|x-y|^2/4t}$$

There are two problems in trying to take m to infinity in the right-hand side of (X.119). The first is that the infinite product of Lebesgue measures does not yield a reasonable measure. Secondly, the product of the kernels p intuitively approaches

$$\exp\left(-\int \dot{\omega}(t)^2\, dt\right) \quad \text{(X.120)}$$

and for arbitrary paths $\dot{\omega}(t)$ is very singular. Fortunately, these two difficulties cancel so long as we lump the two terms together. Thus, our plan is to try to construct a measure μ_{x_0} on a space of paths starting at x_0 so that the right-hand side of (X.119) is just equal to

$$\int_\Omega \prod_{j=1}^{m} e^{-(t/m)V(\omega(jt/m))}\, d\mu_{x_0}(\omega) \quad \text{(X.121)}$$

Since the "zero" of (X.120) will be used to cancel the "infinity" of the infinite product of Lebesgue measures, one should not be surprised that this procedure does not work if (X.120) is replaced by $\exp(-i\int \dot{\omega}(t)^2\, dt)$. This is in fact the case (Problem 64). With this motivation, we begin our construction.

Let $\dot{\mathbb{R}}^n$ be the one point compactification of $\mathbb{R}^n$ and let $\Omega = \bigtimes_{0 \le t} \dot{\mathbb{R}}^n$, the product of uncountably many copies of $\dot{\mathbb{R}}^n$. Then Ω is just the set of all paths in $\dot{\mathbb{R}}^n$ for $t \ge 0$; these are just the paths in $\mathbb{R}^n$ except that they may pass through infinity. We will always consider Ω with the product topology under which it is a compact Hausdorff space by the Tychonoff theorem. This space is so big that the Borel and Baire sets differ. We will always consider regular Borel measures. Now, let $F(x_1, \ldots, x_m)$ be a continuous function on $\bigtimes_{j=1}^{m} \dot{\mathbb{R}}^n$ and fix $t_1 \le \cdots \le t_m$. Then, $\varphi(\omega) = F(\omega(t_1), \ldots, \omega(t_m))$ is a continuous function on Ω. We denote the set of such continuous functions on Ω, for arbitrary m, by $C_{\text{fin}}(\Omega)$ and for such φ we *define*

$$L_{x_0}(\varphi) = \int_{\mathbb{R}^n} \cdots \int_{\mathbb{R}^n} F(x_1, \ldots, x_m) p(x_0, x_1; t_1) p(x_1, x_2; t_2 - t_1) \cdots$$

$$\times\, p(x_{m-1}, x_m; t_m - t_{m-1})\, dx_1 \cdots dx_m \quad \text{(X.122)}$$

L_{x_0} is a well-defined linear functional on $C_{\text{fin}}(\Omega)$ because if F does not depend on x_k, we can use the semigroup property of the heat equation:

$$\int_{\mathbb{R}^n} p(x_{k-1}, x_k; t_k - t_{k-1}) p(x_k, x_{k+1}; t_{k+1} - t_k)\, dx_k$$

$$= p(x_{k-1}, x_{k+1}; t_{k+1} - t_{k-1})$$

to integrate out the variable x_k. Thus $L_{x_0}(\varphi)$ is independent of the representation of φ. Further, $L_{x_0}(1) = 1$ and $L_{x_0}(\varphi) \geq 0$ if $\varphi \geq 0$ since p is positive. Therefore, by the proposition before Theorem IV.14,

$$|L_{x_0}(\varphi)| \leq \sup_{\omega \in \Omega} |\varphi(\omega)|$$

So L_{x_0} is a positive linear functional of norm one on $C_{\text{fin}}(\Omega)$. But, by the Stone–Weierstrass theorem, $C_{\text{fin}}(\Omega)$ is dense in $C(\Omega)$, so L_{x_0} has a unique extension (which we also denote by L_{x_0}) to a positive linear functional of norm one on $C(\Omega)$. Finally, by the Riesz–Markov theorem there is a unique regular Borel measure μ_{x_0} on Ω with $\mu_{x_0}(\Omega) = 1$ so that

$$L_{x_0}(\varphi) = \int_{\Omega} \varphi\, d\mu_{x_0} \qquad \text{for all} \quad \varphi \in C(\Omega)$$

For each x_0, μ_{x_0} is called a **Wiener measure** on Ω and sometimes the whole family of measures $\{\mu_x \mid x \in \mathbb{R}^n\}$ is called Wiener measure.

The measure that we have constructed is a Borel measure. Many interesting sets of paths are Borel subsets of Ω, for example:

Lemma For $0 < \alpha \leq 1$, the set Ω_α of Hölder continuous paths of order α is a Borel subset of Ω.

Proof A path ω is in Ω_α if and only if for all $m < \infty$ there is an M so that

$$|\omega(s) - \omega(t)| \leq M|s - t|^\alpha, \qquad 0 \leq s, t \leq m$$

Therefore,

$$\Omega_\alpha = \bigcap_{m=1}^{\infty} \bigcup_{n=1}^{\infty} \bigcap_{0 \leq s,\, t \leq m} \{\omega \,|\, |\omega(s) - \omega(t)| \leq n|s - t|^\alpha\}$$

Since $\{\omega \,|\, |\omega(s) - \omega(t)| \leq n|s - t|^\alpha\}$ is closed and arbitrary intersections of closed sets are closed, Ω_α is Borel because the last two operations are countable. ∎

The following theorem assures us that the measure μ_{x_0} constructed on the unreasonably large space Ω has support on a set of continuous paths although not on the set of continuously differentiable paths. For a reference, see the Notes.

Theorem X.67 If $0 < \alpha < \frac{1}{2}$, then $\mu_{x_0}(\Omega_\alpha) = 1$ for all $x_0 \in \mathbb{R}^n$. If $\frac{1}{2} \leq \alpha \leq 1$, then $\mu_{x_0}(\Omega_\alpha) = 0$ for all $x_0 \in \mathbb{R}^n$.

We have stated Theorem X.67 because it is used in the proof of the following lemma outlined in Problem 65:

Lemma Let S be a Borel set of Lebesgue measure zero in $\mathbb{R}^n$ and let Ω_S be the set of paths in Ω_α so that $\{t | \omega(t) \in S\}$ has Lebesgue measure zero. Then, for each x in $\mathbb{R}^n$, $\mu_x\{\Omega_S\} = 1$.

We now return to our discussion of the semigroups e^{-tH_0} and $e^{-t(H_0+V)}$. By our construction of μ_x we know that for each continuous function f on $\mathbb{R}^n$, we have, for fixed $\alpha \in (0, \frac{1}{2})$,

$$\int_{\Omega_x} f(\omega(t))\, d\mu_x(\omega) = \int_{\mathbb{R}^n} f(y) p(x, y; t)\, dy \tag{X.123}$$

If f is any measurable function on $\mathbb{R}^n$ so that $f(\cdot)p(x, \cdot, t)$ is integrable, we can approximate f by continuous functions. Then, an application of the dominated convergence theorem shows that (X.123) holds for such f. In particular, (X.123) holds for all $f \in L^2(\mathbb{R}^n)$. But by (IX.31), the right-hand side of (X.123) is just $(e^{-tH_0}f)(x)$, so we have

$$(e^{-tH_0}f)(x) = \int_\Omega f(\omega(t))\, d\mu_x(\omega) \qquad \text{for all } f \in L^2(\mathbb{R}^n)$$

This is the path space integral which gives the free semigroup. We state our interacting path space formulae on $\mathbb{R}^3$. By changing L^2 to L^p with $p > n/2$, it is easy to obtain Feynman–Kac formulae on $\mathbb{R}^n$.

Theorem X.68 (the Feynman–Kac formula) Let V be a real-valued function in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and let $H = H_0 + V$ where $H_0 = -\Delta$. Then for all $f \in L^2(\mathbb{R}^3)$,

$$(e^{-tH}f)(x) = \int_{\Omega_x} f(\omega(t)) \exp\left(-\int_0^t V(\omega(s))\, ds\right) d\mu_x(\omega) \tag{X.124}$$

Proof We prove the theorem in four steps: first for continuous V of compact support, second for V in $L^\infty(\mathbb{R}^3)$, third for $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with $V \leq 0$, and finally for V in the general case. So suppose V is continuous

with compact support. Using (X.119) and (X.122), we have

$$\begin{aligned}
&[(e^{-(t/m)H_0}e^{-(t/m)V})^m f](x) \\
&\quad = \int_{\mathbb{R}^3}\cdots\int_{\mathbb{R}^3} p\left(x, x_m; \frac{t}{m}\right)\cdots p\left(x_2, x_1; \frac{t}{m}\right) \\
&\qquad \times f(x_1)\exp\left(-\sum_{j=1}^{m}\frac{t}{m}V(x_j)\right) dx_1\cdots dx_m \\
&\quad = \int_{\Omega_x}\exp\left(-\frac{t}{m}\sum_{j=1}^{m}V\left(\omega\left(\frac{jt}{m}\right)\right)\right) f(\omega(t))\, d\mu_x(\omega) \qquad \text{(X.125)}
\end{aligned}$$

By the hypotheses on V, $H_0 + V$ is self-adjoint on $D(H_0) = D(H_0) \cap D(V)$, so by the Trotter product formula, $(e^{-(t/m)H_0}e^{-(t/m)V})^m f$ converges to $e^{-tH}f$ in $L^2(\mathbb{R}^3)$. Therefore, there is a subsequence $\{m_j\}$ so that $(e^{-(t/m_j)H_0}e^{-(t/m_j)V})^{m_j}f$ converges to $e^{-tH}f$ almost everywhere. On the other hand, if ω is a continuous path, then $V(\omega(t))$ is continuous in t so

$$\frac{t}{m}\sum_{j=1}^{m}V\left(\omega\left(\frac{jt}{m}\right)\right) \to \int_0^t V(\omega(s))\, ds$$

as $m \to \infty$. Since for each x, almost all (with respect to μ_x) paths are continuous,

$$f(\omega(t))\exp\left(-\frac{t}{n}\sum_{j=1}^{n}V\left(\omega\left(\frac{jt}{n}\right)\right)\right) \to f(\omega(t))\exp\left(-\int_0^t V(\omega(s))\, ds\right)$$

pointwise almost everywhere on Ω_x as $m \to \infty$. Furthermore,

$$\begin{aligned}
\int_{\Omega_x}\left|f(\omega(t))\exp\left(-\frac{t}{n}\sum_{j=1}^{n}V\left(\omega\left(\frac{jt}{n}\right)\right)\right)\right| d\mu_x(\omega) &\le e^{t\max|V|}\int_{\Omega_x}|f(\omega(t))|\, d\mu_x(\omega) \\
&= e^{t\max|V|}(e^{-tH_0}|f|)(x) \\
&< \infty
\end{aligned}$$

for almost all x. Therefore, by the dominated convergence theorem, the right-hand side of (X.125) converges to

$$\int_\Omega f(\omega(t))\exp\left(-\int_0^t V(\omega(s))\, ds\right) d\mu_x(\omega)$$

for almost all x. This proves (X.124) under the special hypotheses that V is continuous with compact support.

Now, suppose that $V \in L^\infty(\mathbb{R}^3)$ and let V_n be a sequence of continuous functions of compact support so that $|V_n(x)| \le \|V\|_\infty$ for all x and $V_n(x) \to V(x)$ pointwise a.e. Then $(H_0 + V_n)$ converges to $H_0 + V$ in strong

resolvent sense, so by Theorem VIII.20, $e^{-t(H_0+V_n)}$ converges strongly to $e^{-t(H_0+V)}$ for each $t \geq 0$. By step one,

$$(e^{-t(H_0+V_n)}f)(x) = \int_{\Omega_x} f(\omega(t)) \exp\left(-\int_0^t V_n(\omega(s))\, ds\right) d\mu_x(\omega) \quad \text{(X.126)}$$

for almost all x and all n. Since $V_n \to V$ pointwise a.e., the lemma implies that for almost all $\omega \in \Omega_x$, $V_n(\omega(t)) \to V(\omega(t))$ pointwise a.e. in t. Therefore, since the V_n and V are uniformly bounded, we have $\int_0^t V_n(\omega(s))\, ds \to \int_0^t V(\omega(s))\, ds$ pointwise a.e. on Ω_x. Thus

$$f(\omega(t)) \exp\left(-\int_0^t V_n(\omega(s))\, ds\right) \to f(\omega(t)) \exp\left(-\int_0^t V(\omega(s))\, ds\right)$$

pointwise a.e. on Ω_x, and now the same dominated convergence theorem argument as in step one shows that the right-hand side of (X.126) converges to the right-hand side of (X.124). On the other hand, as before, a subsequence of the left-hand side of (X.126) converges pointwise a.e. to $e^{-t(H_0+V)}f$ because of the strong convergence. Thus, (X.124) holds in the second case.

Now, suppose that $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with $V \leq 0$. Let $V_n(x) = \max\{V(x), -n\}$. Then V_n is a sequence of decreasing L^∞ functions so that $V_n \xrightarrow{L^2+L^\infty} V$ and $V_n \to V$ pointwise a.e. For each n, the formula (X.124) holds and as $n \to \infty$, $\int_0^t V_n(\omega(s))\, ds \to \int_0^t V(\omega(s))\, ds$ a.e. on Ω_x by the lemma and the monotone convergence theorem. The proof is completed by appealing to the argument in the second case and the monotone convergence theorem.

By obvious modification, the third case holds for V bounded from above and so, appealing again to the monotone convergence theorem, we conclude the proof in the general case. ∎

If $V \in L^2 + (L^\infty)$, then the Feynman–Kac formula implies that

$$\int_\Omega \exp\left(-\int_0^t V(\omega(s))\, ds\right) f(\omega(t))\, d\mu_x(\omega) < \infty$$

for almost all $x \in \mathbb{R}^n$. Therefore

$$-\int_0^t V(\omega(s))\, ds < \infty$$

for almost all ω, for almost all x. Since we can write an arbitrary $V \in L^2 + (L^\infty)$ as a linear combination of its positive and negative parts, we conclude that

$$\int_0^t |V(\omega(s))|\, ds < \infty$$

for almost all ω, for almost all x, if $V \in L^2 + (L^\infty)$.

X.12 Time-dependent Hamiltonians

In this section we prove two existence theorems for the time-dependent Schrödinger equation

$$\frac{d\varphi(t)}{dt} = -iH(t)\varphi(t) \tag{X.127}$$

The investigation of time-dependent problems is important because one sometimes wants to calculate the change in a quantum system in a variety of situations, for example, when an external potential is turned on and then switched off after a short time or when a periodic potential is turned on. We first introduce the analogue of unitary one-parameter groups.

Definition A two-parameter family of unitary operators $U(s, t)$, $s, t \in \mathbb{R}$ which satisfies:

(a) $U(r, s)U(s, t) = U(r, t)$
(b) $U(t, t) = I$
(c) $U(s, t)$ is jointly strongly continuous in s and t

is called a **unitary propagator.**

Theorem X.69 (the Dyson expansion) Let $t \to H(t)$ be a strongly continuous map of $\mathbb{R}$ into the *bounded* self-adjoint operators on a Hilbert space $\mathscr{H}$. Then there is a unitary propagator on $\mathscr{H}$ so that, for all $\psi \in \mathscr{H}$,

$$\varphi_s(t) = U(t, s)\psi$$

satisfies

$$\frac{d}{dt}\varphi_s(t) = -iH(t)\varphi_s(t), \qquad \varphi_s(s) = \psi \tag{X.128}$$

Proof We define

$$U(t, s)\varphi = 1 + \sum_{n=1}^{\infty} (-i)^n \int_s^t \int_s^{t_1} \cdots \int_s^{t_{n-1}} H(t_1) \cdots H(t_n)\varphi \, dt_n \cdots dt_1 \tag{X.129}$$

By the uniform boundedness principle, $H(\tau)$ is uniformly bounded on $[s, t]$, so the nth term on the right is bounded by

$$\frac{|t-s|^n}{n!} \left(\sup_{\tau \in [s,t]} \|H(\tau)\| \right)^n \|\varphi\|$$

so the series on the right converges in the uniform operator topology to $U(t, s)$. Thus $U(t, s)$ is jointly strongly continuous in s and t since this is true of each term on the right. It is trivial to check that $U(t, t) = I$ and that $U(t, s)^* = U(s, t)$; the formula $U(r, s)U(s, t) = U(r, t)$ is proven by multiplying out the series as in the case of unitary groups generated by bounded operators. Thus,

$$U(s, t)U(s, t)^* = I = U(s, t)^*U(s, t)$$

so $U(t, s)$ is unitary. The first statement in (X.128) follows by differentiating the series for $U(t, s)$ term by term and noting that the resulting series converges uniformly. ∎

We remark that the self-adjointness of the $H(t)$ was used only in proving that $U(t, s)$ is unitary; without self-adjointness we can still define $U(t, s)$ as before and use it to construct strong solutions $\varphi_s(t)$.

Although the Dyson expansion requires that $H(t)$ be bounded, by passing to the "interaction representation" we can use it to handle certain cases of the form

$$H(t) = H_0 + V(t)$$

where H_0 is a (possibly unbounded) self-adjoint operator and $t \to V(t)$ satisfies the hypotheses of Theorem X.69. Define

$$\tilde{V}(t) = e^{iH_0t}V(t)e^{-iH_0t}$$

Then $t \to \tilde{V}(t)$ also satisfies the hypotheses of Theorem X.69; we denote the corresponding propagator by $\tilde{U}(t, s)$. If we now set

$$U(t, s) = e^{-itH_0}\tilde{U}(t, s)e^{isH_0}$$

then, at least *formally*, $U(t, s)$ satisfies

$$\frac{d}{dt}U(t, s) = -iH_0 e^{-itH_0}\tilde{U}(t, s)e^{isH_0} + e^{-itH_0}(-i\tilde{V}(t))\tilde{U}(t, s)e^{isH_0}$$

$$= (-iH_0 - iV(t))U(t, s)$$

so $\varphi_s(t) = U(t, s)\psi$ should be a strong solution of

$$\frac{d}{dt}\varphi_s(t) = -i(H_0 + V(t))\varphi_s(t), \qquad \varphi_s(s) = \psi$$

The difficulty is that $H_0\,U(t, s)\psi = H_0\,e^{-itH_0}\tilde{U}(t, s)e^{isH_0}\psi$ may not make sense since $\tilde{U}(t, s)\psi$ may not be in the domain of H_0 even if ψ is. It can be shown (Problem 66) that if $t \to [H_0, V(t)]$ is strongly continuous, then

$\varphi_s(t)$ is in fact a strong solution. This hypothesis is a special case of the more general hypotheses in Theorem X.70 (below); these give rise to strong solutions, so we will not pursue this problem further here. However, we note that for any $\psi \in \mathscr{H}$, $\psi_s(t) = e^{-iH_0t}\tilde{U}(t, s)e^{isH_0}\psi$ is always a "weak" solution in the sense that for any $\eta \in D(H_0)$, $(\eta, \psi_s(t))$ is differentiable and

$$\frac{d}{dt}(\eta, \psi_s(t)) = -i(H_0\eta, \psi_s(t)) - i(V(t)\eta, \psi_s(t))$$

Example 1 The Dyson expansion is important for practical calculations also. Suppose that H_0 is the Hamiltonian of a quantum system and that ψ_k and ψ_ℓ are eigenfunctions of H_0 with corresponding eigenvalues λ_k and λ_ℓ. If the system starts out in state ψ_k, it will stay in ψ_k in the absence of any external potential since $e^{itH_0}\psi_k = e^{it\lambda_k}\psi_k$. However, if an external potential $V(t)$ is turned on for a while the dynamics is given by $e^{-itH_0}\tilde{U}(t, 0)\psi_k$, and if we look at the system at time t the probability that the system will be observed in state ψ_ℓ is $|(\psi_\ell, e^{-itH_0}\tilde{U}(t, 0)\psi_k)|^2$, the transition probability from ψ_k to ψ_ℓ. Using the Dyson expansion we have

$$(\psi_\ell, e^{-itH_0}\tilde{U}(t, 0)\psi_k) = (\psi_\ell, e^{-itH_0}\psi_k) - i\int_0^t (\psi_\ell, e^{-iH_0t}\tilde{V}(t_1)\psi_k)\, dt_1 + \cdots$$

$$= -i\int_0^t e^{-i\lambda_\ell t}e^{-i(\lambda_k - \lambda_\ell)t_1}(\psi_\ell, V(t_1)\psi_k)\, dt_1 + O(t^2)$$

The constant in the term of order t^2 can be easily bounded by estimating the tail of the Dyson expansion, so for small t the above expression allows one to compute upper and lower bounds on the transition probabilities. The reader is asked to compute a specific example in Problem 67.

We come now to the main theorem in this section. Since the proof is the same in the case where $A(t)$ generates a contraction semigroup on a Banach space X, we give the proof in this more general setting. The idea of the proof is very simple and direct. For each positive integer k, we define an approximate propagator $U_k(s, t)$ on $0 \le s \le t \le 1$ by

$$U_k(t, s) = \exp\left(-(t - s)A\left(\frac{i-1}{k}\right)\right) \quad \text{if} \quad \frac{i-1}{k} \le s \le t \le \frac{i}{k} \quad \text{(where } 1 \le i \le k\text{)} \quad \text{(X.130a)}$$

and

$$U_k(t, r) = U_k(t, s)U_k(s, r) \quad \text{if} \quad 0 \le r \le s \le t \le 1 \quad \text{(X.130b)}$$

That is, $U_k(t, s)$ is defined by the constant generator $A((i-1)/k)$ for s and t in the small intervals $[(i-1)/k, i/k]$ and by the product formula when s and t are not both in the same small interval. We will show that under suitable hypotheses, $U_k(t, s)$ converges to a propagator $U(t, s)$ so that $\varphi_s(t) = U(t, s)\psi$ solves $d\varphi_s(t)/dt = -A(t)\varphi_s(t)$. To see what these hypotheses should be we compute formally

$$\begin{aligned}(U_k(t,0) - U_n(t,0))A(0)^{-1}\varphi &= [U_n(t,s)U_k(s,0)A(0)^{-1}\varphi]_{s=0}^{s=t} \\ &= \int_0^t \frac{d}{ds}\,(U_n(t,s)U_k(s,0)A(0)^{-1}\varphi)\,ds \\ &= \int_0^t U_n(t,s)\left\{A\left(\frac{[ns]}{n}\right) - A\left(\frac{[ks]}{k}\right)\right\} \\ &\quad \times A\left(\frac{[ks]}{k}\right)^{-1} A\left(\frac{[ks]}{k}\right) U_k(s,0)A(0)^{-1}\varphi\,ds\end{aligned} \tag{X.131}$$

where $[r]$ always denotes the largest integer less than or equal to r. The fact that $A([ns]/n)$ can be written to the right of $U_n(t, s)$ follows by writing $U_n(t, s)$ as a product if t and s are not in the same small interval. Thus to show that the left-hand side of (X.131) is small, it suffices that $A(t)A(s)^{-1} - I$ be small when $|t - s|$ is small and that $A(t)U_k(t, 0)A(s)^{-1}$ be bounded. We thus define

$$C(t, s) = A(t)A(s)^{-1} - I$$

and state:

Theorem X.70 Let X be a Banach space and let I be an open interval in $\mathbb{R}$. For each $t \in I$, let $A(t)$ be the generator of a contraction semigroup on X so that $0 \in \rho(A(t))$ and

(a) The $A(t)$ have a common domain D (from which it follows by the closed graph theorem that $A(t)A(s)^{-1}$ is bounded).

(b) For each $\varphi \in X$, $(t-s)^{-1}C(t, s)\varphi$ is uniformly strongly continuous and uniformly bounded in s and t for $t \neq s$ lying in any fixed compact subinterval of I.

(c) For each $\varphi \in X$, $C(t)\varphi \equiv \lim_{s \uparrow t} (t-s)^{-1}C(t, s)\varphi$ exists uniformly for t in each compact subinterval and $C(t)$ is bounded and strongly continuous in t.

Then for all $s \leq t$ in any compact subinterval of I and any $\varphi \in X$,

$$U(t, s)\varphi = \lim_{k \to \infty} U_k(t, s)\varphi$$

exists uniformly in s and t. Further, if $\psi \in D$, then $\varphi_s(t) \equiv U(t, s)\psi$ is in D for all t and satisfies

$$\frac{d}{dt}\varphi_s(t) = -A(t)\varphi_s(t), \qquad \varphi_s(s) = \psi$$

and $\|\varphi_s(t)\| \leq \|\psi\|$ for all $t \geq s$.

We make two remarks. First, the hypothesis that $0 \in \rho(A(t))$ is usually not a strong restriction. If we can find a $z_0 \in \rho(A(t))$ for all t and if the operators $B(t) = A(t) - z_0$ satisfy the hypothesis, then $\tilde{U}(t, s) = U(t, s)e^{(s-t)z_0}$ is a propagator for $A(t)$ if $U(t, s)$ is the propagator for $B(t)$. In particular, when $A(t)$ is i times a self-adjoint operator, we can use this trick. Secondly, it is sufficient to prove the existence of the propagator for $s, t \in [0, 1]$ since we can then use the same procedure to extend to $[1, 2]$ and so forth. We begin by showing that the hypotheses imply the boundedness of $A(t)U(t, s)A(s)^{-1}$.

Lemma For $s, t \in [0, 1]$ define $W_k(t, s) = A(t)U_k(t, s)A(s)^{-1}$. Then $\|W_k(t, s)\| \leq M_1$ independent of s, t, and k.

Proof Fix s, t, and k. Since $U_k(t, s)$: $D \to D$, $W_k(t, s)$ is well defined on X. Letting $\psi \in X$, we write $W_k(t, s)$ as

$$\begin{aligned}
W_k(t, s)\psi &= A(t)U_k\left(t, \frac{[kt]}{k}\right)U_k\left(\frac{[kt]}{k}, \frac{[kt]-1}{k}\right)\cdots U_k\left(\frac{[ks]+1}{k}, s\right)A(s)^{-1}\psi \\
&= A(t)A\left(\frac{[kt]}{k}\right)^{-1}U_k\left(t, \frac{[kt]}{k}\right)A\left(\frac{[kt]}{k}\right)A\left(\frac{[kt]-1}{k}\right)^{-1}\cdots \\
&\quad \times A\left(\frac{[ks]}{k}\right)^{-1}U_k\left(\frac{[ks]+1}{k}, s\right)A\left(\frac{[ks]}{k}\right)A(s)^{-1}\psi \\
&= \left(I + C\left(t, \frac{[kt]}{k}\right)\right)\left\{U_k(t, s) + \sum_{ku=[ks]+1}^{[kt]} U_k(t, u)C\left(u, u - \frac{1}{k}\right)U_k(u, s)\right. \\
&\quad + \sum_{kv=[ks]+1}^{[kt]} U_k(t, v)C\left(v, v - \frac{1}{k}\right)\sum_{ku=[ks]+1}^{[kt]} U_k(v, u) \\
&\quad \left.\times C\left(u, u - \frac{1}{k}\right)U_k(u, s) + \cdots\right\}\left(I + C\left(\frac{[ks]}{k}, s\right)\right)\psi \\
&= \left(I + C\left(t, \frac{[tk]}{k}\right)\right)\{U_k(t, s) + W_k^1(t, s) + W_k^2(t, s) + \cdots\} \\
&\quad \times \left(I + C\left(\frac{[ks]}{k}, s\right)\right)\psi
\end{aligned}$$

where

$$W_k^1(t, s) = \sum_{ku=[ks]+1}^{[kt]} U_k(t, s)C\left(u, u - \frac{1}{k}\right)U_k(u, s)$$

and

$$W_k^{m+1}(t, s) = \sum_{ku=[ks]+1}^{[kt]} U_k(t, s)C\left(u, u - \frac{1}{k}\right)W_k^m(u, s) \qquad \text{(X.132)}$$

Let

$$M_2 = \sup_{t \neq s} \|(t - s)^{-1}C(t, s)\|$$

Then

$$\left\|C\left(u, u - \frac{1}{k}\right)\psi\right\| \leq \frac{M_2}{k}\|\psi\|$$

so from (X.132) we have

$$\|W_k^1(t, s)\psi\| \leq (t - s)M_2\|\psi\| \qquad \text{and} \qquad \|W_k^m(t, s)\psi\| \leq \frac{(t - s)^m}{m!}M_2^m\|\psi\|$$

Therefore

$$\|W_k(t, s)\| \leq \left(1 + \frac{M_2}{k}\right)^2\left(1 + \sum_{m=1}^{\infty}\frac{(t - s)^m}{m!}M_2^m\right)\|\psi\|$$

We have repeatedly used the fact that $\|U_k(r_1, r_2)\psi\| \leq \|\psi\|$ since each $A(t)$ generates a contraction semigroup. ∎

Proof of Theorem X.70 Let $\varphi \in D$. Since $U_k(r, s)\varphi \in D$ for $r \geq s$ and

$$U_k(t, s)\varphi = e^{-(t-[kt]/k)A([kt]/k)}U_k\left(\frac{[kt]}{k}, s\right)\varphi$$

we see that $U_k(t, s)$ is strongly differentiable in t except when $t = j/k$, and letting $A(0)\varphi = \psi$,

$$\begin{aligned}\frac{d}{dt}U_k(t, s)\varphi &= -A\left(\frac{[kt]}{k}\right)U_k(t, s)\varphi \\ &= -A\left(\frac{[kt]}{k}\right)A(t)^{-1}A(t)U_k(t, s)A(s)^{-1}A(s)A(0)^{-1}\psi \\ &= -A\left(\frac{[kt]}{k}\right)A(t)^{-1}W_k(t, s)A(s)A(0)^{-1}\psi\end{aligned}$$

Thus, since $\|W_k(t, s)\|$ is uniformly bounded and $C(t, s)$ is strongly continuous, we see that $dU_k(t, s)\varphi/dt$ is bounded and strongly continuous

except at $t = j/k$. A similar proof shows that the same conclusion holds for

$$\frac{d}{ds} U_k(t, s)\varphi = -U_k(t, s)A\left(\frac{[ks]}{k}\right)\varphi$$

when $s \neq j/k$. Thus if $k > n$,

$$\begin{aligned}
&(U_k(t, s) - U_n(t, s))A(0)^{-1}\psi \\
&\quad = [U_n(t, r)U_k(r, s)]_{r=s}^{r=t} A(0)^{-1}\psi \\
&\quad = \int_s^t \frac{d}{dr}\{U_n(t, r)U_k(r, s)A(0)^{-1}\psi\}\, dr \qquad \text{(X.133)} \\
&\quad = \int_s^t U_n(t, r)\left\{A\left(\frac{[rn]}{n}\right) - A\left(\frac{[rk]}{k}\right)\right\}A\left(\frac{[rn]}{n}\right)^{-1} A\left(\frac{[rn]}{n}\right)U_k(r, s)A(0)^{-1}\psi\, dr \\
&\quad = \int_s^t U_n(t, r)C\left(\frac{[rn]}{n}, \frac{[rk]}{k}\right)\left\{1 + C\left(\frac{[rn]}{n}, r\right)\right\}W_k(r, s)\{1 + C(s, 0)\}\psi\, dr
\end{aligned}$$

Since

$$\left\|C\left(\frac{[rk]}{k}, \frac{[rn]}{n}\right)\right\| \leq 2\left|\frac{[rk]}{k} - \frac{[rn]}{n}\right| \sup_{s \neq t}|t - s|^{-1}\|C(t, s)\|$$

and $U_n(t, r)$, $C([rn]/n, r)$, $C(s, 0)$, and $W_k(r, s)$ (by the lemma) are all uniformly bounded independent of r, s, t, n, and k, we see that the strong limit of $U_k(t, s)$ exists uniformly in t and s. Since $U_k(t, s)$ is uniformly bounded

$$U(t, s)\varphi \equiv \lim_{k \to \infty} U_k(t, s)\varphi$$

exists for all $\varphi \in X$ and $U(t, s)$ is a bounded-operator-valued function and is uniformly strongly jointly continuous. We remark that the integral (X.133) is really a sum of integrals over the intervals where the derivative exists.

A similar proof shows that

$$W(t, s)\varphi \equiv \lim_{k \to \infty} W_k(t, s)\varphi$$

exists boundedly and uniformly in t and s and that $W(t, s)$ is a bounded-operator-valued function which is jointly strongly continuous. Thus, if $\varphi \in D$, $U_k(t, s)\varphi \to U(t, s)\varphi$ and

$$\begin{aligned}
A(t)U_k(t, s)\varphi &= W_k(t, s)A(s)\varphi \\
&\xrightarrow[k \to \infty]{} W(t, s)A(s)\varphi
\end{aligned}$$

Since $A(t)$ is closed, this implies that $U(t, s)\varphi \in D$ and $A(t)U(t, s)\varphi = W(t, s)A(s)\varphi$. Furthermore

$$\begin{aligned} U(t, s)\varphi - \varphi &= \lim_{k\to\infty} (U_k(t, s)\varphi - \varphi) \\ &= \lim_{k\to\infty} \int_s^t \frac{d}{dr} U_k(r, s)\varphi \, dr \\ &= \lim_{k\to\infty} -\int_s^t A\left(\frac{[rk]}{k}\right) U_k(r, s)\varphi \, dr \\ &= -\lim_{k\to\infty} \int_s^t A\left(\frac{[rk]}{k}\right) A(r)^{-1}A(r)U_k(r, s)A(s)^{-1}A(s)\varphi \, dr \\ &= -\int_s^t W(r, s)A(s)\varphi \, dr \end{aligned}$$

Since $W(r, s)$ is strongly continuous,

$$\frac{d}{dt} U(t, s)\varphi = -W(t, s)A(s)\varphi = -A(t)U(t, s)\varphi$$

which concludes the proof of Theorem X.70. ∎

Example 2 We can easily apply this result to the heat equation with time-dependent sources and sinks proportional to the temperature. Let $q(x, t)$ be a bounded real-valued continuously differentiable function on $\mathbb{R}^{n+1}$ so that $\partial q(x, t)/\partial t$ is bounded. Let M be the bound of q and set

$$A(t) = -\Delta + q(x, t) + (M + 1)$$

on $C_\infty(\mathbb{R}^n)$. From Examples 3 and 4 in Section X.8 we know that $A(t)$ is the generator of a contraction semigroup on $C_\infty(\mathbb{R}^n)$ and that $D(A(t)) = D(-\Delta)$ for all t. The reader can easily check (Problem 68) that the hypotheses on $q + M + 1$ imply that the conditions of Theorem X.70 are satisfied. Thus for each $\psi \in D(-\Delta)$ there is a function $\tilde{\varphi}(x, t)$ so that for each t, $\tilde{\varphi}(x, t) \in D(-\Delta)$ and

$$\frac{d}{dt} \tilde{\varphi}(x, t) = \Delta\tilde{\varphi}(x, t) - q(x, t)\tilde{\varphi}(x, t) - (M + 1)\tilde{\varphi}(x, t)$$

$$\tilde{\varphi}(x, 0) = \psi(x)$$

If we now define $\varphi(x, t) = e^{(M+1)t}\tilde{\varphi}(x, t)$, then $\varphi(x, t)$ satisfies

$$\frac{d}{dt} \varphi(x, t) = \Delta\varphi(x, t) - q(x, t)\varphi(x, t)$$

$$\varphi(x, 0) = \psi(x)$$

Notice that $U_k(t, s)$ is positivity preserving for each k since it is the product of positivity-preserving transformations (see Example 4 in Section X.8). Thus $U(t, s)$ is positivity preserving since it is the strong limit of the $U_k(t, s)$. Therefore, given any nonnegative initial data $\psi \in C_\infty(\mathbb{R})$, the solution $\varphi(x, t) = e^{(M+1)t}U(t, s)\psi$ will remain nonnegative corresponding to our intuition about heat flow.

Finally, we apply Theorem X.70 to the quantum mechanical case.

Theorem X.71 Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and suppose that $t \to V_1(t)$ and $t \to V_2(t)$ are continuously differentiable $L^2(\mathbb{R}^3)$-valued and $L^\infty(\mathbb{R}^3)$-valued functions respectively. Let $V(t) = V_1(t) + V_2(t)$ and set $H(t) = H_0 + V(t)$. Then there is a unitary propagator $U(t, s)$ on $L^2(\mathbb{R}^3)$ so that for each $\psi \in D(H_0)$, $\varphi_s(t) = U(t, s)\psi$ is strongly differentiable and satisfies

$$\frac{d}{dt}\varphi_s(t) = -iH(t)\varphi_s(t), \qquad \varphi_s(s) = \psi \tag{X.134}$$

Proof We will construct a unitary propagator for each finite interval $[-T, T]$. By Theorem X.15, $H_0 + V(t)$ is self-adjoint on $D(-\Delta)$ for each t. Further, since $V_1(t)$ and $V_2(t)$ are uniformly bounded in L^2 and L^∞ norm respectively, we can find a constant $D \geq 0$ so that $H_0 + V(t) + D \geq \frac{1}{2}$ for all $t \in [-T, T]$. Thus $i(H_0 + V(t) + D)$ and $-i(H_0 + V(t) + D)$ generate contraction semigroups for each t and $(\pm i(H_0 + V(t) + D))^{-1}$ exists for $t \in [-T, T]$. Further, the hypotheses on $t \to V_1(t)$ and $t \to V_2(t)$ imply that $i(H_0 + V(t) + D)$ and $-i(H_0 + V(t) + D)$ satisfy the hypotheses (b) and (c) of Theorem X.70. Let $U^+(t, s)$ and $U^-(t, s)$ be the corresponding propagators. Since U_k^+ and U_k^- are unitary for each k, U^+ and U^- are unitary. Now define

$$\tilde{U}(t, s) = \begin{cases} U^+(t, s), & s \leq t \\ U^-(s, t), & t \leq s \end{cases}$$

and

$$U(t, s) = e^{iD(t-s)}\tilde{U}(t, s) \quad \blacksquare$$

We conclude this section with a brief outline of a method due to J. Howland for turning time-dependent problems into time-independent problems. In classical mechanics, Hamilton's equations for a system with Hamiltonian function $H(p_1, \ldots, p_n, q_1, \ldots, q_n, t)$ are

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad -\frac{dp_i}{dt} = \frac{\partial H}{\partial q_i}, \qquad i = 1, \ldots, n \tag{X.135}$$

If H depends on t, energy is not conserved by such a system, but we can set up a corresponding energy conserving system by introducing t as a coordinate and the energy E of the external source as its conjugate momentum. The new Hamiltonian is

$$h(\mathbf{p}, \mathbf{q}, t, E) = E + H(\mathbf{p}, \mathbf{q}, t)$$

so if we denote by σ the new time variable, Hamilton's equations read

$$\begin{aligned} \frac{dq_i}{d\sigma} &= \frac{\partial H}{\partial p_i}, \qquad -\frac{dp_i}{d\sigma} = \frac{\partial H}{\partial q_i}, \qquad i = 1, \ldots, n \\ \frac{dt}{d\sigma} &= \frac{\partial h}{\partial E} = 1, \qquad -\frac{dE}{d\sigma} = \frac{\partial H}{\partial t} \end{aligned} \tag{X.136}$$

This set of equations is equivalent to (X.135).

We can reformulate the quantum-mechanical problem similarly. Let $H(t)$ be a family of self-adjoint operators on a Hilbert space $\mathscr{H}$ and set $\mathscr{H}_1 = L^2(\mathbb{R}; \mathscr{H})$, the Hilbert space of strongly measurable $\mathscr{H}$-valued functions $f(\cdot)$ on $\mathbb{R}$ such that $\int_{-\infty}^{\infty} \|f(t)\|_{\mathscr{H}}^2 \, dt < \infty$. If we now define h on $\mathscr{H}_1$ by

$$(hf)(t) = -i\frac{d}{dt}f(t) + H(t)f(t)$$

there should be (according to the classical analogy) a correspondence between the solutions of

$$\frac{d}{d\sigma}\varphi(\sigma) = -ih\varphi(\sigma)$$

on $\mathscr{H}_1$ and the solutions of the time-dependent problem (X.134) on $\mathscr{H}$. Suppose that $U(t, s)$ is a unitary propagator on $\mathscr{H}$. Then

$$(\hat{U}(\sigma)f)(t) \equiv U(t, t-\sigma)f(t-\sigma) \tag{X.137}$$

is a strongly continuous unitary group on $\mathscr{H}_1$ (Problem 69). Notice that this means that if T_σ is the group on $\mathscr{H}_1$ which acts by $(T_\sigma f)(t) = f(t+\sigma)$, then $\hat{U}(\sigma)T_\sigma$ acts on $\mathscr{H}_1$ by multiplication by an operator-valued function. Conversely, one can prove that to each strongly continuous unitary group $\hat{U}(\sigma)$ on $\mathscr{H}$, so that $\hat{U}(\sigma)T_\sigma$ is multiplication by an operator-valued function, there corresponds a unique unitary propagator $U(t, s)$ on $\mathscr{H}$ so that (X.137) holds. Thus, we have a correspondence between unitary propagators on $\mathscr{H}$ and certain strongly continuous one-parameter unitary groups on $\mathscr{H}_1$. Notice that $\hat{U}(\sigma)$ will always be strongly differentiable on a dense set in $\mathscr{H}_1$ by Stone's theorem, but that $U(t, s)$ need not be strongly

differentiable on $\mathscr{H}$. Thus, we have a method of proving the existence of propagators in situations where we might not expect strong differentiability, i.e., situations where we cannot use Theorem X.70. This propagator formally solves

$$\frac{d}{dt}U(t,s)\psi = -iH(t)U(t,s)\psi$$

Example 3 We will consider again the case $H(t) = H_0 + V(t)$ where H_0 is a self-adjoint operator on $\mathscr{H}$ and $t \to V(t)$ is a strongly continuous map from $\mathbb{R}$ to the bounded operators on $\mathscr{H}$. To make things easier, we will assume that $\|V(t)\|$ is uniformly bounded on all of $\mathbb{R}$. As before we let $\tilde{V}(t) = e^{iH_0t}V(t)e^{-iH_0t}$. Let $\hat{\tilde{V}}$ be the operator on $L^2(\mathbb{R};\mathscr{H})$ which acts by $(\hat{\tilde{V}}f)(t) = \tilde{V}(t)f(t)$ and let $C_0^1(\mathbb{R};\mathscr{H})$ denote the continuously differentiable $\mathscr{H}$-valued functions on $\mathbb{R}$ with compact support. Then it is not hard to check that $i^{-1}\,d/dt$ is essentially self-adjoint on $C_0^1(\mathbb{R};\mathscr{H})$. Since $\hat{\tilde{V}}$ is a bounded operator, $i^{-1}\,d/dt + \hat{\tilde{V}}$ is also essentially self-adjoint on $C_0^1(\mathbb{R};\mathscr{H})$ and it is possible to show that $\exp(-i\sigma(i^{-1}\,d/dt + \hat{\tilde{V}}))T_\sigma$ operates by multiplication by an operator-valued function. Thus by the correspondence theorem mentioned above, there is a strongly continuous propagator $\tilde{U}(t,s)$ on $\mathscr{H}$ so that

$$\left(\exp\left(-i\sigma\left(\frac{1}{i}\frac{d}{dt} + \hat{\tilde{V}}\right)\right)f\right)(t) = \tilde{U}(t,t-\sigma)f(t-\sigma)$$

One can easily check that this $\tilde{U}$ is just the propagator arising from applying the Dyson expansion to $t \to \tilde{V}(t)$. Now, let $\hat{W}$ act on $L^2(\mathbb{R};\mathscr{H})$ by $(\hat{W}f)(t) = e^{-iH_0t}f(t)$. Then $\hat{W}$ is unitary so

$$\hat{W}\exp\left(-i\sigma\left(\frac{1}{i}\frac{d}{dt} + \hat{\tilde{V}}\right)\right)\hat{W}^{-1}$$

is again a strongly continuous unitary group on $L^2(\mathbb{R};\mathscr{H})$ and clearly

$$\left(\hat{W}\exp\left(-i\sigma\left(\frac{1}{i}\frac{d}{dt} + \hat{\tilde{V}}\right)\right)\hat{W}^{-1}f\right)(t) = e^{-itH_0}\tilde{U}(t,t-\sigma)e^{i(t-\sigma)H_0}f(t-\sigma)$$

So $U(t,s) = e^{-itH_0}\tilde{U}(t,s)e^{isH_0}$ is the propagator on $\mathscr{H}$ which formally solves

$$\frac{d}{dt}U(t,s) = -i(H_0 + V(t))U(t,s)$$

since the generator of $\hat{W}\exp(-i\sigma(i^{-1}\,d/dt + \hat{\tilde{V}}))\hat{W}^{-1}$ is $i^{-1}d/dt + H_0 + \hat{V}$.

X.13 Classical nonlinear wave equations

A thorough discussion of nonlinear partial differential equations is outside the scope of this book. However, we want to describe some of the functional analytic techniques which are useful in studying these classical problems. We will use the nonlinear Klein–Gordon equation as a motivating example. Suppose that $m, \lambda > 0$, and let two functions f and g on $\mathbb{R}^3$ be given. The problem is to prove the existence and study the behavior of a function $u(x, t)$ satisfying

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \Delta u + m^2 u &= -\lambda |u|^2 u \\ u(x, 0) &= f(x) \\ \frac{\partial u}{\partial t}(x, 0) &= g(x) \end{aligned} \tag{X.138}$$

In this section we treat the existence, uniqueness, and smoothness of solutions of (X.138). In Section XII.13, we develop a scattering theory for (X.138). We are treating the Klein–Gordon problem for complex-valued functions u. If the initial data f and g are real valued, then u will be real valued for all t (Problem 71) and thus satisfies

$$u_{tt} - \Delta u + m^2 u = -\lambda u^3 \tag{X.139}$$

This equation is the classical analogue of the φ^4 quantum field theory equation discussed in Section X.7.

Classical field theories like those described by (X.139) are formally in the form of Hamiltonian systems. If we let

$$H(u, v) = \frac{1}{2} \int \left(v(x)^2 + (\nabla u(x))^2 + m^2 u(x)^2 + \frac{\lambda}{2} u(x)^4 \right) d^3x$$

then (X.139) is formally equivalent to

$$u_t(x) = \frac{\delta H}{\delta v(x)} = v(x)$$

$$v_t(x) = -\frac{\delta H}{\delta u(x)} = (\Delta - m^2) u(x) - \lambda (u(x))^3$$

where we have integrated by parts to obtain

$$\int (\nabla u(x))^2 \, d^3x = -\int u(x) \, \Delta u(x) \, d^3x$$

This suggests that, as in classical Hamiltonian systems with a finite number of degrees of freedom, the total energy should be conserved. That is, if u is a sufficiently smooth solution of (X.139) which falls off fast enough at infinity to justify integrations by parts and differentiation under the integral sign, then $H(u, u_t)$ should be time independent. Such a conservation law will be crucial for the *global* existence theory of (X.138) and (X.139) and will distinguish between the cases $\lambda > 0$ and $\lambda < 0$. If $\lambda > 0$, then as time develops both u and ∇u are prevented from getting large, since neither can get large without $H(u, u_t)$ getting large. On the other hand if $\lambda < 0$, then both u and ∇u can get large in such a way that their contributions to $H(u, u_t)$ cancel. Thus, one expects global solutions to exist if $\lambda > 0$ and we prove this by exploiting conservation of energy. If $\lambda < 0$, we expect that for some initial data global solutions will not exist. This situation is analogous to the situation with the ordinary differential equation

$$m\ddot{q}(t) = \lambda q^3(t)$$

Since the energy $\frac{1}{2}m\dot{q}^2 + \frac{1}{4}\lambda q^4$ is conserved, the solution cannot get to infinity in finite time if $\lambda > 0$, so global solutions exist; but if $\lambda < 0$, the solution does get to infinity in finite time.

Since the techniques which we have developed in this chapter so far apply to differential equations of first order in t, we rewrite (X.138) as a first-order system:

$$\frac{\partial v}{\partial t} - \Delta u + m^2 u = -\lambda |u|^2 u$$

$$\frac{\partial u}{\partial t} = v$$

$$u(x, 0) = f(x)$$

$$v(x, 0) = g(x)$$

or

$$\dot{\varphi}(t) - \begin{pmatrix} 0 & I \\ \Delta - m^2 & 0 \end{pmatrix} \varphi(t) = J(\varphi(t)) \tag{X.140}$$

$$\varphi(x, 0) = \begin{pmatrix} f(x) \\ g(x) \end{pmatrix}$$

where

$$\varphi = \begin{pmatrix} u \\ v \end{pmatrix} \quad \text{and} \quad J(\varphi) = \begin{pmatrix} 0 \\ -\lambda |u|^2 u \end{pmatrix}$$

From now on we write column vectors as row vectors. Our plan is to formulate (X.140) as a Hilbert space problem and then prove a general Hilbert space theorem guaranteeing existence and uniqueness. Let $B \geq mI$ be the positive square root of a strictly positive self-adjoint operator B^2 on a Hilbert space $\mathscr{H}$. (In our case $\mathscr{H} = L^2(\mathbb{R}^3)$ and $B^2 = -\Delta + m^2$.) Since B^2 is closed, the domain of B, $D(B)$, is a Hilbert space under the inner product (Bu, Bu). We will denote by $\mathscr{H}_B$ the direct sum $\mathscr{H}_B \equiv D(B) \oplus \mathscr{H}$ with the inner product

$$(\langle u, v\rangle, \langle u, v\rangle)_B \equiv (Bu, Bu) + (v, v)$$

Let

$$A = i\begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix} \tag{X.141}$$

Then it is easy to check that A is a symmetric operator on $\mathscr{H}_B$ with domain $D \equiv D(B^2) \oplus D(B)$ and that A is closed since B and B^2 are closed. Now, defining $\cos(tB)$ and $\sin(tB)$ by the functional calculus, we set

$$W(t) = \begin{pmatrix} \cos(tB) & B^{-1}\sin(tB) \\ -B\sin(tB) & \cos(tB) \end{pmatrix}$$

Then $W(t)$ is a strongly continuous unitary group on $\mathscr{H}_B$. Furthermore, if $u \in D$, the strong derivative of $W(t)u$ exists at zero and equals $-iA$ and $W(t)$ takes D into itself. Thus, by Theorem VIII.11, the generator of $W(t)$ is essentially self-adjoint on D. Since A is closed, A is self-adjoint on D and is the infinitesimal generator of $W(t)$. We summarize in a proposition.

Proposition Let B be a strictly positive self-adjoint operator on a Hilbert space $\mathscr{H}$. Then $W(t)$ is a strongly continuous one-parameter unitary group on $\mathscr{H}_B$ whose infinitesimal generator

$$A = i\begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix}$$

is self-adjoint on $D = D(B^2) \oplus D(B)$.

We can now formulate an abstract version of (X.140). Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ (no longer necessarily of the form (X.141)) and suppose that J is a nonlinear mapping from $D(A)$ to $\mathscr{H}$. The problem is to find conditions on J guaranteeing that for each $\varphi_0 \in D(A)$, there is a unique $\mathscr{H}$-valued function $\varphi(t)$ on $[0, \infty)$ satisfying

$$\begin{aligned} \frac{d\varphi}{dt} &= -iA\varphi + J(\varphi) \\ \varphi(0) &= \varphi_0 \end{aligned} \tag{X.142}$$

The technique of proof is to reformulate (X.142) as an integral equation

$$\varphi(t) = e^{-iAt}\varphi_0 + \int_0^t e^{-i(t-s)A} J(\varphi(s))\, ds \tag{X.143}$$

and prove the existence of unique local solutions of (X.143) by the contraction mapping principle. Our conditions on J will be strong enough to guarantee that any solution of (X.143) is automatically a solution of (X.142). It is possible to weaken the conditions on J so that one obtains solutions of (X.143) but not of (X.142) because the solution is not necessarily strongly differentiable.

Theorem X.72 (local existence) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J a mapping from $D(A)$ to $D(A)$ which satisfies:

(H_0) $\quad \|J(\varphi)\| \leq C(\|\varphi\|)\|\varphi\|$

(H_1) $\quad \|AJ(\varphi)\| \leq C(\|\varphi\|, \|A\varphi\|)\|A\varphi\|$

(H_0^L) $\quad \|J(\varphi) - J(\psi)\| \leq C(\|\varphi\|, \|\psi\|)\|\varphi - \psi\|$

(H_1^L) $\quad \|A(J(\varphi) - J(\psi))\| \leq C(\|\varphi\|, \|A\varphi\|, \|\psi\|, \|A\psi\|)\|A\varphi - A\psi\|$

for all $\varphi, \psi \in D(A)$ where each constant C is a monotone increasing (everywhere finite) function of the norms indicated. Then, for each $\varphi_0 \in D(A)$ there is a $T > 0$ so that (X.142) has a unique continuously differentiable solution for $t \in [0, T)$. For each set of the form $\{\varphi \mid \|\varphi\| \leq a, \|A\varphi\| \leq b\}$, T can be chosen uniformly for all φ_0 in the set.

Proof Let X_T be the set of $D(A)$-valued functions on $[0, T)$ for which $\varphi(t)$ and $A\varphi(t)$ are continuous and

$$\|\varphi(\cdot)\|_T \equiv \sup_{t \in [0, T)} \|\varphi(t)\| + \sup_{t \in [0, T)} \|A\varphi(t)\| < \infty$$

Since A is a closed operator, X_T with the norm $\|\varphi(\cdot)\|_T$ is a Banach space. Choose some fixed $\varepsilon > 0$. Let $\varphi_0 \in D(A)$ be given and let $X_{T,\varepsilon,\varphi_0}$ consist of those $\varphi(\cdot)$ in X_T with $\varphi(0) = \varphi_0$ and $\|\varphi(\cdot) - e^{-iAt}\varphi_0\|_T \leq \varepsilon$. We will show that the map

$$(S\varphi)(t) = e^{-iAt}\varphi_0 + \int_0^t e^{-iA(t-s)} J(\varphi(s))\, ds \tag{X.144}$$

is a contraction on $X_{T,\varepsilon,\varphi_0}$ if T is small enough. We denote by C_ε any of the constants in the hypotheses with arguments $\|\varphi_0\| + \varepsilon$ and $\|A\varphi_0\| + \varepsilon$. Suppose that $\varphi(\cdot) \in X_{T,\varepsilon,\varphi_0}$; then

$$\begin{aligned}
&\|e^{-iA(t-(s+h))}J(\varphi(s+h)) - e^{-iA(t-s)}J(\varphi(s))\| \\
&\quad \leq \|J(\varphi(s+h)) - J(\varphi(s))\| + \|(e^{-iAh} - I)J(\varphi(s))\| \\
&\quad \leq C_\varepsilon\|\varphi(s+h) - \varphi(s)\| + \|(e^{-iAh} - I)J(\varphi(s))\|
\end{aligned}$$

so $e^{-iA(t-s)}J(\varphi(s))$ is a continuous $\mathscr{H}$-valued function of s. A similar proof shows that $Ae^{-iA(t-s)}J(\varphi(s))$ is also continuous. Thus, the right-hand side of (X.144) can be defined using the Riemann integral, and if

$$\eta_n(t) \equiv \sum_{m=1}^{n} \frac{1}{n} e^{-i(t-(m/n)t)A} J\left(\varphi\left(\frac{m}{n}t\right)\right)$$

and

$$\eta(t) \equiv \int_0^t e^{-i(t-s)A} J(\varphi(s))\, ds$$

then $\eta_n(t) \to \eta(t)$ as $n \to \infty$. Now, by the hypotheses on J, each $\eta_n(t) \in D(A)$, so

$$\begin{aligned} A\eta_n(t) &= \sum_{m=1}^{n} \frac{1}{n} e^{-i(t-(m/n)t)A} AJ\left(\varphi\left(\frac{m}{n}t\right)\right) \\ &\to \int_0^t e^{-i(t-s)A} AJ(\varphi(s))\, ds \end{aligned}$$

Therefore, $\eta(t) \in D(A)$ and

$$A\int_0^t e^{-i(t-s)A} J(\varphi(s))\, ds = \int_0^t e^{-i(t-s)A} AJ(\varphi(s))\, ds \tag{X.145}$$

Further,

$$\begin{aligned} \|A\eta(t+h) - A\eta(t)\| &\le \left\| \int_t^{t+h} e^{-iA(t-s)} e^{-iAh} AJ(\varphi(s))\, ds \right\| \\ &\quad + \left\| \int_0^t (e^{-ihA} - I) e^{-iA(t-s)} AJ(\varphi(s))\, ds \right\| \\ &\le hC_\varepsilon \|\varphi\|_T + \int_0^t \|(e^{-ihA} - I)AJ(\varphi(s))\|\, ds \end{aligned}$$

The integrand in the second term converges to zero as $h \to 0$ for each s and by the hypotheses on J, the integrand is uniformly bounded. Thus, by the dominated convergence theorem the right-hand side converges to zero as $h \to 0$, so $A\eta(t)$ is continuous and similarly, $\eta(t)$ is continuous. Further, exactly the same kind of estimates as above show that for any $\varphi(\cdot)$, $\psi(\cdot) \in X_{T,\varepsilon,\varphi_0}$, we have

$$\|(S\varphi)(t) - e^{-iAt}\varphi_0\| \le C_\varepsilon T \sup_{t \in [0,T)} \|\varphi(t)\|$$

$$\|A(S\varphi)(t) - Ae^{-iAt}\varphi_0\| \le C_\varepsilon T \sup_{t \in [0,T)} \|A\varphi(t)\|$$

$$\|(S\varphi)(t) - (S\psi)(t)\| \le C_\varepsilon T \sup_{t \in [0,T)} \|\varphi(t) - \psi(t)\|$$

$$\|A[(S\varphi)(t) - (S\psi)(t)]\| \le C_\varepsilon T \sup_{t \in [0,T)} \|A\varphi(t) - A\psi(t)\|$$

Thus, for T small enough, S is a contraction on $X_{T,\varepsilon,\varphi_0}$ so, by Theorem V.18, S has a unique fixed point $\varphi(\cdot)$ in $X_{T,\varepsilon,\varphi_0}$ which satisfies (X.143).

Now, suppose that $\tilde{\varphi}$ is a continuously differentiable $D(A)$-valued solution of (X.142) on the interval $[0, \tilde{T})$ with $\tilde{\varphi}(0) = \varphi_0$. By the differential equation, $A\tilde{\varphi}(t)$ is continuous, so $\tilde{\varphi}(t) \in X_{T,\varepsilon,\varphi_0}$ for t in some interval $[0, T_0)$. Since $\tilde{\varphi}$ obeys (X.143), $\varphi(t) = \tilde{\varphi}(t)$ for $t < T_0$. Let T_1 be the sup of such T_0. Then since $X_{T,\varepsilon,\varphi_0}$ is closed, $\tilde{\varphi}(T_1) \in X_{T,\varepsilon,\varphi_0}$. Now, if $T_1 < T$, then since $\tilde{\varphi}(T_1) = \varphi(T_1)$ the same argument as above shows that $\tilde{\varphi}(t) = \varphi(t)$ for some small interval of $T_1 \leq t < T_2 < T$ which contradicts the maximality of T_1. Thus $T_1 \geq T$, so $\tilde{\varphi}(t) = \varphi(t)$ for $t \in [0, T)$. That is, any strong solution of (X.142) on $[0, T)$ equals $\varphi(t)$.

To prove the strong differentiability of $\varphi(t)$ we write

$$\frac{\varphi(t+h) - \varphi(t)}{h} = \left(\frac{e^{-iAh} - I}{h}\right) e^{-iAt}\varphi_0 + \frac{1}{h}\int_t^{t+h} e^{-iA(t-s)} e^{-ihA} J(\varphi(s))\, ds$$
$$+ \int_0^t e^{-iA(t-s)} \left(\frac{e^{-ihA} - I}{h}\right) J(\varphi(s))\, ds \qquad \text{(X.146)}$$

Since $\varphi_0 \in D(A)$ the first term converges to $-iAe^{-iAt}\varphi_0$ as $h \to 0$ and since the integrand of the second term is continuous, it converges to $J(\varphi(t))$. The integrand of the third term converges to $e^{-iA(t-s)}(-iAJ(\varphi(s)))$ for each s and

$$\left\| \frac{e^{-ihA} - I}{h} J(\varphi(s)) \right\| \leq \|AJ(\varphi(s))\| \leq C\|A\varphi_0\| + \varepsilon$$

so the integrand is uniformly bounded. Thus, by the dominated convergence theorem the third term converges as $h \to 0$ to $\int_0^t e^{-iA(t-s)}\,(-iAJ(\varphi(s)))\, ds$ which by (X.145) equals $-iA\int_0^t e^{-iA(t-s)} J(\varphi(s))\, ds$. Therefore $\varphi(t)$ is strongly differentiable for $t \in [0, T)$ and satisfies (X.142). ∎

Uniqueness in the above theorem actually holds in a considerably stronger sense (Problem 72). We remark that the hypotheses H_j in the above and the following theorem follow from the hypotheses H_j^L. We state them separately for easy comparison with the hypotheses of Theorem X.74.

Theorem X.73 (local smoothness)

(a) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J a mapping which takes $D(A^j)$ into $D(A^j)$ for all $1 \leq j \leq n$ and which satisfies (for $j = 0, 1, \ldots, n$)

(H_j) $\quad \|A^j J(\varphi)\| \leq C(\|\varphi\|, \ldots, \|A^j\varphi\|)\|A^j\varphi\|$

(H_j^L) $\quad \|A^j(J(\varphi) - J(\psi))\|$
$$\leq C(\|\varphi\|, \|\psi\|, \ldots, \|A^j\varphi\|, \|A^j\psi\|)\|A^j\varphi - A^j\psi\|$$

for all $\varphi, \psi \in D(A^j)$ where each constant C is a monotone increasing (everywhere finite) function of all its variables. Then for each $\varphi_0 \in D(A^n)$, $n \geq 1$, there is a T_n so that (X.142) has a unique solution $\varphi(t)$ for $t \in [0, T_n)$ with $\varphi(t) \in D(A^n)$ for all $t \in [0, T_n)$. For each set of the form $\{\varphi \mid \|A^j\varphi\| \leq a_j, j = 0, \ldots, n\}$, T can be chosen uniformly for φ_0 in the set.

(b) In addition to the hypotheses in (a) assume that for each $j < n$, J has the following property: If a solution φ is j times strongly continuously differentiable with $\varphi^{(k)}(t) \in D(A^{n-k})$ and $A^{n-k}\varphi^{(k)}(t)$ is continuous for all $k \leq j$, then $J(\varphi(t))$ is j times differentiable, $d^jJ(\varphi(t))/dt^j \in D(A^{n-j-1})$, and $A^{n-j-1}\, d^jJ(\varphi(t))/dt^j$ is continuous. Then the solution given in part (a) is n times strongly differentiable in t and $d^j\varphi(t)/dt^j \in D(A^{n-j})$.

Proof The proof of part (a) is essentially the same as the proof of Theorem X.72 except that we take $X^{(n)}_{T_n, \varepsilon, \varphi_0}$ to be the set of functions $\varphi(\cdot)$ on $[0, T_n)$ so that $\varphi(t), \ldots, A^n\varphi(t)$ are strongly continuous and

$$\sum_{j=0}^{n} \sup_{t \in [0, T)} \|A^j\varphi(t) - e^{-iAt}A^j\varphi_0\| \leq \varepsilon$$

Then one proves that S is a contraction as before.

Part (b) is proven by induction. We know from part (a) that $\varphi(t)$ is strongly continuously differentiable and $\varphi'(t) = -iA\varphi(t) + J(\varphi(t))$. By the same arguments as in Theorem X.72,

$$\begin{aligned} A\varphi(t) &= Ae^{-iAt}\varphi_0 + A\int_0^t e^{-iA(t-s)}J(\varphi(s))\, ds \\ &= e^{-iAt}A\varphi_0 + \int_0^t e^{-iA(t-s)}AJ(\varphi(s))\, ds \end{aligned}$$

and from this it follows (using another argument in Theorem X.72; see (X.146)) that $A\varphi(t)$ is strongly continuously differentiable. Therefore by the hypotheses on J, $J(\varphi(t))$ is strongly continuously differentiable, $dJ(\varphi(t))/dt \in D(A^{n-2})$, and $A^{n-2}\, dJ(\varphi(t))/dt$ is continuous. Thus, $\varphi'(t)$ is strongly differentiable,

$$\begin{aligned} \varphi''(t) &= -A\varphi'(t) + \frac{d}{dt}J(\varphi(t)) \\ &= (-iA)^2\varphi(t) - iAJ(\varphi(t)) + \frac{d}{dt}J(\varphi(t)) \end{aligned}$$

$\varphi''(t) \in D(A^{n-2})$, and $A^{n-2}\varphi''(t)$ is continuous. We now repeat the argument again ($dJ(\varphi(t))/dt$ is differentiable by hypothesis since we now know that $\varphi(t)$ is twice continuously differentiable) to conclude that $\varphi(t)$ is three times strongly differentiable and so forth. ∎

Notice that the solution $\varphi(t)$ guaranteed by Theorem X.73 will generally exist on a smaller interval than the solution in Theorem X.72 since $T_n \leq T$. But by uniqueness these solutions must coincide on $[0, T_n)$. We now come to the question of whether the solution exists for all $t \geq 0$. In general this will depend on detailed properties of the nonlinear terms and not just estimates; at the end of the section we give an example where global existence does not hold. Below, we prove that if $\|\varphi(t)\|$ is a priori bounded and if we have slightly stronger estimates, then global solutions exist. Later, we will see that the conserved energy for the nonlinear Klein–Gordon equation is $\frac{1}{2}\|\varphi(t)\|^2 + \frac{1}{4}\lambda \int |u(t, x)|^4 \, d^3x$ so that $\|\varphi(t)\|$ is a priori bounded.

Lemma 1 Let A and J satisfy the hypotheses of part (a) of Theorem X.73 except that the hypotheses (H_j) are replaced by the slightly strongly hypotheses:

$$(H'_j) \qquad \|A^j J(\varphi)\| \leq C(\|\varphi\|, \ldots, \|A^{j-1}\varphi\|)\|A^j\varphi\|$$

for $1 \leq j \leq n$ (i.e., the constant does not depend on $\|A^j\varphi\|$). Let $[0, T_n)$ be a finite interval on which a solution φ of (X.142) exists with $A^j\varphi(t)$ strongly continuous on $[0, T_n)$ for each $0 \leq j \leq n$. Then, if $\|\varphi(t)\|$ is bounded on $[0, T_n)$ so is $\|A^j\varphi(t)\|$ for each $0 < j \leq n$.

Proof Since $\varphi(t)$ satisfies the differential equation on $[0, T_n)$ we have for $t \in [0, T_n)$:

$$\varphi(t) = e^{-iAt}\varphi_0 + \int_0^t e^{-iA(t-s)}J(\varphi(s))\, ds$$

As before we can take A inside the integral to conclude that

$$A\varphi(t) = e^{-iAt}A\varphi_0 + \int_0^t e^{-iA(t-s)}AJ(\varphi(s))\, ds$$

so,

$$\|A\varphi(t)\| \leq \|A\varphi_0\| + \int_0^t C(\|\varphi(s)\|)\|A\varphi(s)\|\, ds$$

By hypothesis, $\|\varphi(s)\|$ is bounded on $[0, T_n)$ so there is a constant K_1 so that

$$\|A\varphi(t)\| \leq \|A\varphi_0\| + K_1 \int_0^t \|A\varphi(s)\|\, ds$$

for all $t \in [0, T_n)$. Thus by iteration we conclude that

$$\|A\varphi(t)\| \leq \|A\varphi_0\| e^{K_1 t}$$

for all $t \in [0, T_n)$ so $\|A\varphi(t)\|$ is bounded on $[0, T_n)$. Now that we know that $\|\varphi(t)\|$ and $\|A\varphi(t)\|$ are bounded, we can use (H_2') and the same argument to conclude that $\|A^2\varphi(t)\|$ is bounded and so forth. ∎

Let $\overline{T}_n$ be the sup of the numbers T_n so that a solution $\varphi(t)$ of (X.142) exists on $[0, T_n)$ with $A^j\psi(t)$ continuous for each $j = 0, 1, \ldots, n$. By local uniqueness, each of these solutions coincide wherever their intervals of existence overlap, so the solution given by part (a) of Theorem X.73 may be extended to $[0, \overline{T}_n)$ which is called the **A^n-maximal interval** of existence of the solution.

Theorem X.74 (global existence and smoothness) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and n a positive integer. Let J be a mapping which takes $D(A^j)$ into $D(A^j)$ for all $1 \le j \le n$ and which satisfies (for all $0 \le j \le n$)

$$(H_0) \qquad \|J(\varphi)\| \le C(\|\varphi\|)\|\varphi\|$$

$$(H_j') \qquad \|A^jJ(\varphi)\| \le C(\|\varphi\|, \ldots, \|A^{j-1}\varphi\|)\|A^j\varphi\|, \qquad j = 1, \ldots, n$$

$$(H_j^L) \qquad \|A^j(J(\varphi) - J(\psi))\| \le C(\|\varphi\|, \|\psi\|, \ldots, \|A^j\varphi\|, \|A^j\psi\|)\|A^j\varphi - A^j\psi\|, \qquad j = 0, \ldots, n$$

for all $\varphi, \psi \in D(A^j)$ where each constant C is a monotone increasing (everywhere finite) function of all its variables. Let $\varphi_0 \in D(A^n)$ and suppose that on any finite interval of existence the solution $\varphi(t)$ guaranteed by part (a) of Theorem X.73 has the property that $\|\varphi(t)\|$ is bounded from above. Then there is a strongly differentiable $D(A^n)$-valued function $\varphi(t)$ on $[0, \infty)$ that satisfies

$$\begin{aligned} \varphi'(t) &= -iA\varphi(t) + J(\varphi(t)) \\ \varphi(0) &= \varphi_0 \end{aligned} \tag{X.142}$$

Further, if J satisfies the hypotheses of part (b) of Theorem X.73, then $\varphi(t)$ is n-times strongly differentiable and $d^j\varphi(t)/dt^j \in D(A^{n-j})$.

Proof Let $[0, \overline{T}_n)$ be the A^n-maximal interval of existence of the solution $\varphi(t)$ and suppose $\overline{T}_n < \infty$. By hypothesis, we know that $\|\varphi(t)\|$ is bounded on $[0, \overline{T}_n)$. This implies by Lemma 1 that $\|A^j\varphi(t)\|$ is bounded on $[0, \overline{T}_n)$ for all $0 \le j \le n$. Now, the length of the interval T_n over which one can use the contraction mapping principle depends only on the constants $C(\|\varphi_0\| + \varepsilon, \ldots, \|A^n\varphi_0\| + \varepsilon)$. Since they are bounded on $[0, \overline{T}_n)$, we can extend the solution $\varphi(t)$ across $\overline{T}_n$ if we choose as initial point a t_0 close enough to $\overline{T}_n$. Since this violates the maximality of $\overline{T}_n$, we conclude that $\overline{T}_n = \infty$. The rest of the statements of the theorem follow immediately from Theorem X.73. ∎

Corollary Let A and J satisfy the hypotheses of the above theorem for each $n = 0, 1, \ldots$ and suppose that J satisfies the hypotheses of part (b) of Theorem X.73. Then for each $\varphi_0 \in \bigcap_{j=1}^{\infty} D(A^j)$, (X.142) has a unique solution $\varphi(t)$ so that $\varphi(t)$ is infinitely often strongly differentiable and each derivative is in $\bigcap_{j=1}^{\infty} D(A^j)$.

We make several remarks. First, since e^{itA} is a group and all our estimates are independent of the sign of t, Theorem X.74 shows the existence of a solution for negative t as long as $\|\varphi(t)\|$ is a priori bounded on finite negative intervals also. Suppose that we have the hypothesis

$$(\mathscr{H}_0^1) \qquad \|J(\varphi) - J(\psi)\| \leq C(\|\varphi\|, \|\psi\|)\|\varphi - \psi\| \qquad \varphi, \psi \in \mathscr{H}$$

and the a priori boundedness condition of Theorem X.47. Then by the ideas above, we can construct global solutions of the integral equation (X.143). Let M_t be the mapping

$$M_t : \varphi(0) \to \varphi(t)$$

where $\varphi(t)$ is the solution of (X.143). Then $\{M_t\}_{t \in (-\infty, \infty)}$ is a one-parameter group of everywhere defined nonlinear mappings on $\mathscr{H}$. M_t is strongly continuous since $\|\varphi(t) - \varphi(0)\| \to 0$ as $t \to 0$. It is often important to know that for each t, M_t is a continuous operator on $\mathscr{H}$ since in applications, this says that the solutions of differential equations depend continuously on the initial data. Notice that since M_t is in general nonlinear, it is not sufficient to prove that M_t is bounded on bounded sets.

Theorem X.75 Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J a nonlinear mapping on $\mathscr{H}$ satisfying $(\mathscr{H}_0^1)$. Suppose that for all k, T, solutions of (X.143) are a priori bounded, uniformly for all $\|\varphi(0)\| \leq k$, $0 < t < T$. Then each M_t is uniformly continuous on balls in $\mathscr{H}$.

Proof Let k, T be given and let $b_T(k)$ be the corresponding uniform bound. Suppose that $\|\varphi_1(0)\| \leq k$, $\|\varphi_2(0)\| \leq k$ and let $\varphi_1(t)$, $\varphi_2(t)$ be the corresponding solutions of (X.143). Then, for $t < T$,

$$\|\varphi_1(t) - \varphi_2(t)\| \leq \|\varphi_1(0) - \varphi_2(0)\| + \int_0^t \|J(\varphi_1(s)) - J(\varphi_2(s))\|\, ds$$

$$\leq \|\varphi_1(0) - \varphi_2(0)\| + C(b(k), b(k)) \int_0^t \|\varphi_1(s) - \varphi_2(s)\|\, ds$$

so,

$$\|\varphi_1(t) - \varphi_2(t)\| \leq \|\varphi_1(0) - \varphi_2(0)\| \exp(C(b(k), b(k))t) \quad \blacksquare$$

With stronger hypothesis on J one can obtain a stronger conclusion; see Problem 80.

* * *

We now return to our motivating example, the nonlinear Klein–Gordon equation on $\mathbb{R}^3$. In that case, $B = (-\Delta + m^2)^{1/2}$ on $L^2(\mathbb{R}^3)$, $\mathscr{H} = D(B) \oplus L^2(\mathbb{R}^3)$, and

$$A = i\begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix}$$

In the following, the symbol $\|\cdot\|$ will always denote the norm

$$\|\langle u, v\rangle\|^2 = \|Bu\|_2^2 + \|v\|_2^2$$

on $\mathscr{H}$ and $\|\cdot\|_p$ will denote the ordinary L^p norm on $\mathbb{R}^3$. We reformulated the Klein–Gordon equation (X.138) as

$$\begin{aligned} \varphi'(t) &= -iA\varphi(t) + J(\varphi(t)) \\ \varphi(0) &= \varphi_0 \end{aligned} \tag{X.147}$$

where $\varphi(t) = \langle u(t), v(t)\rangle$, $\varphi_0 = \langle f(x), g(x)\rangle$, $J(\varphi(t)) = \langle 0, -\lambda|u(t)|^2 u(t)\rangle$, and we showed in the proposition that A is self-adjoint on $D(B^2) \oplus D(B)$. In order to apply the abstract theory to this case we must verify that J has the right properties. No new techniques are required but just an appropriate use of Hölder's inequality, the Plancherel theorem, and a Sobolev estimate. We proceed by a series of lemmas. In all the following calculations, various universal constants will be denoted by K.

Lemma 2 Let $u \in C_0^\infty(\mathbb{R}^3)$. Then $\|u\|_6 \le K\|Bu\|_2$.

Proof Denote $\partial u(x)/\partial x_i$ by u_{x_i}. Then by the fundamental theorem of calculus,

$$|u(x)|^4 \le 4 \int |u_{x_i} u^3| \, dx_i$$

where the integral is taken over the line where x_j is held fixed for $j \neq i$. Thus

$$|u(x)|^6 \le K\left(\int |u_{x_1} u^3| \, dx_1\right)^{1/2} \left(\int |u_{x_2} u^3| \, dx_2\right)^{1/2} \left(\int |u_{x_3} u^3| \, dx_3\right)^{1/2}$$

so by integrating both sides (by iterating the integrals) and using the Schwarz inequality, one obtains

$$\begin{aligned}\int_{\mathbb{R}^3}|u|^6\,dx &\le K\left(\int_{\mathbb{R}^3}|u_{x_1}u^3|\,dx\right)^{1/2}\left(\int_{\mathbb{R}^3}|u_{x_2}u^3|\,dx\right)^{1/2}\left(\int_{\mathbb{R}^3}|u_{x_3}u^3|\,dx\right)^{1/2}\\ &\le K\left(\int_{\mathbb{R}^3}|u|^6\,dx\right)^{3/4}\left(\int_{\mathbb{R}^3}|u_{x_1}|^2\,dx\right)^{1/4}\\ &\quad\times\left(\int_{\mathbb{R}^3}|u_{x_2}|^2\,dx\right)^{1/4}\left(\int_{\mathbb{R}^3}|u_{x_3}|^2\,dx\right)^{1/4}\end{aligned}$$

From this one easily obtains

$$\begin{aligned}\left(\int_{\mathbb{R}^3}|u|^6\,dx\right)^{1/6} &\le K(\|u_{x_1}\|_2+\|u_{x_2}\|_2+\|u_{x_3}\|_2)\\ &= K(\|k_1\hat{u}\|_2+\|k_2\hat{u}\|_2+\|k_3\hat{u}\|_2)\\ &\le K\|(\textstyle\sum k_i^2+m^2)^{1/2}\hat{u}\|_2\\ &= K\|Bu\|_2\ \blacksquare\end{aligned}$$

Lemma 3 Suppose that $u_1, u_2, u_3 \in D(B)$. Then

$$\|u_1u_2u_3\|_2 \le K\|Bu_1\|_2\|Bu_2\|_2\|Bu_3\|_2 \tag{X.148}$$

Proof Let $u \in D(B)$. Since B is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$, we can find a sequence of $C_0^\infty(\mathbb{R}^3)$ functions u_n so that $u_n \xrightarrow{L^2} u$ and $Bu_n \xrightarrow{L^2} Bu$, and by passing to a subsequence if necessary, we may assume u_n converges pointwise to u also. But

$$\begin{aligned}\|u_n^3-u_m^3\|_2 &= \|(u_n-u_m)(u_n^2+u_nu_m+u_m^2)\|_2\\ &\le K\|u_n-u_m\|_6\|(u_n^2+u_nu_m+u_m^2)\|_3\\ &\le K\|u_n-u_m\|_6(\|u_n\|_6^2+\|u_n\|_6\|u_m\|_6+\|u_m\|_6^2)\\ &\le K\|Bu_n-Bu_m\|_2(\|Bu_n\|_2^2+\|Bu_n\|_2\|Bu_m\|_2+\|Bu_m\|_2^2)\end{aligned}$$

so $\{u_n^3\}$ is Cauchy in L^2 and since it converges pointwise to u^3 we have $u^3 \in L^2$. Taking the limit in the inequality we obtain

$$\|u\|_6^3 = \|u^3\|_2 \le K\|Bu\|_2^3$$

The statement of the lemma now follows by applying Hölder's inequality twice. ∎

Lemma 4 For all $\varphi_1, \varphi_2 \in \mathscr{H}$, J satisfies

$$\|J(\varphi_1)\| \le K\|\varphi_1\|^3$$
$$\|J(\varphi_1) - J(\varphi_2)\| \le C(\|\varphi_1\|, \|\varphi_2\|)\|\varphi_1 - \varphi_2\|$$

Proof Let $\varphi_i = \langle u_i, v_i\rangle$. Then, by Lemma 3,

$$\|J(\varphi_1)\| = \|\lambda u_1^2 \bar{u}_1\|_2 \le K\|Bu_1\|_2^3 \le K\|\varphi_1\|^3$$

and (by the calculation in Lemma 3)

$$\begin{aligned}\|J(\varphi_1) - J(\varphi_2)\| &= \|\lambda(u_1^2\bar{u}_1 - u_2^2\bar{u}_2)\|_2 \\ &\le K\|B(u_1 - u_2)\|_2(\|Bu_1\|_2^2 + \|Bu_1\|_2\|Bu_2\|_2 + \|Bu_2\|_2^2) \\ &\le K\|\varphi_1 - \varphi_2\|(\|\varphi_1\|^2 + \|\varphi_1\|\,\|\varphi_2\| + \|\varphi_2\|^2)\end{aligned}$$

which proves the lemma. ∎

Lemma 5 Let $\varphi_1, \varphi_2 \in D(A)$, then

$$\|AJ(\varphi_1)\| \le K\|\varphi_1\|^2\|A\varphi_1\|$$
$$\|A(J(\varphi_1) - J(\varphi_2))\| \le C(\|\varphi_1\|, \|\varphi_2\|, \|A\varphi_1\|, \|A\varphi_2\|)\|A\varphi_1 - A\varphi_2\|$$

Proof Let $\varphi_i = \langle u_i, v_i\rangle$ where $u_i \in D(B^2)$, $v_i \in D(B)$. We compute

$$\|Bu_{x_i}\|_2^2 = \|(\textstyle\sum k_i^2 + m^2)^{1/2} k_i \hat{u}\|_2^2 \le \|(\sum k_i^2 + m^2)\hat{u}\|_2^2 = \|B^2 u\|_2^2$$

so, by Lemma 3,

$$\|(u^2\bar{u})_{x_i}\|_2 = \|2uu_{x_i}\bar{u} + u^2\bar{u}_{x_i}\|_2 \le K\|Bu\|_2^2\|Bu_{x_i}\|_2 \le K\|Bu\|_2^2\|B^2u\|_2$$

Thus,

$$\begin{aligned}\|AJ(\varphi_1)\|^2 = \lambda^2\|Bu_1^2\bar{u}_1\|_2^2 &= \lambda^2 \sum_{i=1}^{3} \|(u_1^2\bar{u}_1)_{x_i}\|_2^2 + \lambda^2 m^2\|u_1^2\bar{u}_1\|_2^2 \\ &\le K(\|Bu_1\|_2^4\|B^2u_1\|_2^2 + m^2\|Bu_1\|_2^6) \\ &\le K\|Bu_1\|_2^4\|B^2u_1\|_2^2 \\ &\le K\|\varphi_1\|^4\|A\varphi_1\|^2\end{aligned}$$

which proves the first inequality. To prove the second, we compute by Lemma 3 and the above,

$$\begin{aligned}\tfrac{1}{4}\|(u_1^2\bar{u}_1 - u_2^2\bar{u}_2)_{x_i}\|_2^2 &\le \|u_1^2(\bar{u}_1 - \bar{u}_2)_{x_i}\|_2^2 + \|(u_1^2 - u_2^2)(\bar{u}_2)_{x_i}\|_2^2 \\ &\quad + \|2(u_1)_{x_i}(|u_1|^2 - |u_2|^2)\|_2^2 + \|2(u_1 - u_2)_{x_i}|u_2|^2\|_2^2 \\ &\le K(\|Bu_1\|_2^4\|B^2(u_1 - u_2)\|_2^2 \\ &\quad + \|B^2u_2\|_2^2\|B(u_1 + u_2)\|_2^2\|B^2(u_1 - u_2)\|_2^2) \\ &\le K(\|\varphi_1\|^4\|A(\varphi_1 - \varphi_2)\|^2 \\ &\quad + \|A\varphi_2\|^2(\|\varphi_1\| + \|\varphi_2\|)\|A(\varphi_1 - \varphi_2)\|^2)\end{aligned}$$

Therefore

$$\begin{aligned}\|A(J(\varphi_1) - J(\varphi_2))\|^2 &= \lambda^2 \|B(u_1^2 \bar{u}_1 - u_2^2 \bar{u}_2)\|_2^2 \\ &= \lambda^2 \sum_{i=1}^{3} \|(u_1^2 \bar{u}_1 - \bar{u}_2 u_2^2)_{x_i}\|_2^2 + m^2 \lambda^2 \|u_1^2 \bar{u}_1 - u_2^2 \bar{u}_2\|_2^2 \\ &\leq C(\|\varphi_1\|, \|\varphi_2\|, \|A\varphi_2\|)\|A(\varphi_1 - \varphi_2)\|^2 \\ &\quad + C(\|\varphi_1\|, \|\varphi_2\|)\|A(\varphi_1 - \varphi_2)\|^2\end{aligned}$$

which proves the lemma. We have several times used the inequality $\|Bu\|_2 \leq K\|B^2 u\|_2$. ∎

The last two lemmas and Theorem X.72 guarantee the local existence of a solution to (X.138). To get global existence we need:

Lemma 6 Let $u(x, t)$ be the solution of (X.138) on an interval $[0, T)$ where $u(x, 0) = f(x) \in D(B^2)$ and $u_t(x, 0) = g(x) \in D(B)$. Then

$$E(t) \equiv \frac{1}{2} \int \left\{ |Bu(x, t)|^2 + |u_t(x, t)|^2 + \frac{\lambda}{2} |u(x, t)|^4 \right\} d^3x$$

is independent of t.

Proof Let $\varphi(t) = \langle u(x, t), u_t(x, t) \rangle$. Since $\varphi(t) \in D(A)$ for each $t \in [0, T)$, we have $u(\cdot, t) \in D(B^2)$ and $u_t(x, t) \in D(B)$ for each $t \in [0, T)$. Further, since $\varphi(t)$ is strongly differentiable, u and u_t are strongly differentiable as $L^2(\mathbb{R}^3)$-valued functions and

$$\begin{aligned}\left\| B\left(\frac{u(t + h) - u(t)}{h} - u_t(t) \right) \right\|_2 &\to 0 \\ \left\| \frac{u_t(t + h) - u_t(t)}{h} - u_{tt}(t) \right\|_2 &\to 0\end{aligned} \tag{X.149}$$

as $h \to 0$. From this it follows that the first two terms in $E(t)$ are differentiable. To see that the third term is differentiable we use Lemma 2 and Hölder's inequality to conclude that

$$\begin{aligned}&\left\| u\left(\frac{u(t + h) - u(t)}{h} - u_t(t) \right) \right\|_2 \\ &\quad \leq \|u\|_2^{1/2} \|Bu\|_2^{1/2} \left\| B\left(\frac{u(t + h) - u(t)}{h} - u_t(t) \right) \right\|_2\end{aligned}$$

From this and (X.149) above, it follows that $u(t, x)^2$ is strongly differentiable. Therefore

$$\int |u(t, x)|^4 \, dx = (u^2(t), u^2(t))_2$$

is differentiable. Thus, $E(t)$ is differentiable and

$$\begin{aligned} E'(t) &= \frac{1}{2}(Bu_t, Bu) + \frac{1}{2}(u_{tt}, u_t) + \frac{\lambda}{2}(uu_t, u^2) \\ &\quad + \frac{1}{2}(Bu, Bu_t) + \frac{1}{2}(u_t, u_{tt}) + \frac{\lambda}{2}(u^2, uu_t) \\ &= \frac{1}{2}(u_t, B^2u + u_{tt} + \lambda|u|^2u) + \frac{1}{2}(B^2u + u_{tt} + \lambda|u|^2u, u_t) \\ &= 0 \end{aligned}$$

on account of the differential equation for u. ∎

Theorem X.76a Let $\lambda > 0$, $m > 0$ and suppose

$$f \in D(-\Delta + m^2), \qquad g \in D((-\Delta + m^2)^{1/2})$$

Then there exists a unique function $u(x, t)$, $t \in \mathbb{R}$, $x \in \mathbb{R}^3$, so that $t \mapsto u(\cdot, t)$ is a twice strongly differentiable $L^2(\mathbb{R}^3)$-valued function of t, $u(\cdot, t) \in D(-\Delta + m^2)$ for all t, $u(x, 0) = f(x)$, $u_t(x, 0) = g(x)$, and

$$u_{tt} - \Delta u + m^2 u = -\lambda|u|^2u \tag{X.138}$$

Moreover, for each t, the map $\langle f, g\rangle \mapsto \langle u(\cdot, t), u_t(\cdot, t)\rangle$ is continuous.

Proof Lemmas 4 and 5 show that J satisfies the hypotheses (H_0'), (H_1'), (H_0^{L}), and (H_1^{L}) of Theorem X.72. Thus, a unique local solution $\varphi(t) = \langle u(x, t), u_t(x, t)\rangle$ exists on an interval $[0, T)$. By Lemma 6, $E(t)$ is constant, so for all $t \in [0, T)$,

$$\begin{aligned} \frac{1}{2}\|\varphi(t)\|^2 &\le \frac{1}{2}\|\varphi(t)\|^2 + \frac{\lambda}{4}\int_{\mathbb{R}^3} |u(x, t)|^4 \, d^3x \\ &= E(t) = E(0) \end{aligned}$$

Thus $\|\varphi(t)\|$ is bounded on $[0, T)$, so by Theorem X.74 the solution exists for all $t \ge 0$. By solving the equation with initial data $\langle f, -g\rangle$ we obtain a solution for $t \le 0$. The other statements also follow immediately from part (a) of Theorem X.73 and Theorem X.75. In verifying the hypotheses of Theorem X.75, it is necessary to note that the nonlinear term in the energy can be bounded by the square of the free energy. ∎

From a classical point of view, Theorem X.75 is not completely satisfactory. We would like to know that if we start out with initial data with a certain degree of smoothness the solution will remain that smooth. It is for this reason that one needs Theorem X.73. We will sketch the proof of the C^∞ result.

Theorem X.76b Suppose that the initial data f and g in Theorem X.76a are both in $C_0^\infty(\mathbb{R})$. Then the solution $u(x, t)$ of (X.138) is in $C^\infty(\mathbb{R}^4)$.

Proof First one proves the higher order estimates (H_n') and (H_n^{L}) for all $n > 1$. The proofs are straightforward and use exactly the same ideas that we used in proving the cases $n = 0$ and $n = 1$ in Lemmas 5 and 6. Then one verifies for each n the hypotheses on J given in part (b) of Theorem X.73. To show what is involved we will do the case $n = 2$. Suppose that $\varphi(t)$ solves (X.147), $\varphi(t) \in D(A^2)$, $\varphi'(t) \in D(A)$, and $A\varphi'(t)$ is continuous in t. We must show that $J(\varphi(t))$ is strongly differentiable. Now, $\varphi(t) = \langle u(t), u'(t)\rangle$ and by the hypotheses on φ, $u(t) \in D(B^3)$ and $u'(t) \in D(B^2)$. We can write

$$\frac{1}{h}\left(J(\varphi(t+h)) - J(\varphi(t))\right) = -\lambda\left\langle 0, \frac{|u(t+h)|^2 u(t+h) - |u(t)|^2 u(t)}{h}\right\rangle$$

as the sum of three terms one of which is

$$-\lambda\left\langle 0, |u(t)|^2\left(\frac{u(t+h) - u(t)}{h}\right)\right\rangle$$

and the other two are similar. By Lemma 4,

$$\left\| |u(t)|^2\left[\left(\frac{u(t+h) - u(t)}{h}\right) - u'(t)\right]\right\|_2$$

$$\leq K\|Bu(t)\|_2^2 \left\| B\left[\frac{u(t+h) - u(t)}{h} - u'(t)\right]\right\|_2$$

But, since $\varphi(t)$ is strongly differentiable, the right-hand side converges to zero. The same argument works for the other two terms so we conclude that $J(\varphi(t))$ is strongly differentiable,

$$(J(\varphi(t)))' = -\lambda\langle 0, 2u\bar{u}u' + u^2\bar{u}'\rangle$$

$(J(\varphi(t)))' \in D(A^{2-1-1}) = \mathscr{H}$ by Lemma 4 again, and $J(\varphi(t))'$ is continuous. By exactly such arguments as these one verifies the hypotheses of part (b) of Theorem X.73.

Now, since $f, g \in C_0^\infty(\mathbb{R}^3)$, $\varphi_0 = \langle f, g\rangle$ is contained in $\bigcap_{n=1}^\infty D(A^n)$. Therefore, by the Corollary to Theorem X.73, we see that $\varphi(t)$ is infinitely often strongly differentiable and for each j, the jth derivative $\varphi^{(j)}(t)$ is in $\bigcap_{n=1}^\infty D(A^n)$ for all t. All that remains is to prove that there is a function, u, C^∞ in the classical sense, so that if we view $u(\cdot, t)$ as a vector-valued function of t, then $\varphi(t) = \langle u(x, t), u_t(x, t)\rangle$. Now $u(t)$, the first component of $\varphi(t)$ is locally an element of $L^2(\mathbb{R}, L^2(\mathbb{R}^3)) = L^2(\mathbb{R}^4)$ (see Section II.4). The L^2 derivatives of u in the time direction are clearly the distributional derivatives (since $C_0^\infty \subset L^2$), and since $\partial^k u/\partial t^k \in \bigcap_{n=1}^\infty D(B^n)$ by the above argument, the distributional derivatives of u are L^2 for all orders. By Sobolev's lemma (Theorem IX.24), u is C^∞ in the classical sense. ∎

Finally, to complete our analysis of the nonlinear Klein-Gordon equation we show that the solution propagates at speed one. In particular, the solution u of the last theorem has the property that $u(\cdot, t) \in C_0^\infty(\mathbb{R}^n)$ for all t.

Theorem X.77 Let $f \in D(-\Delta + m^2)$ and $g \in D((-\Delta + m^2)^{1/2})$ and suppose that f and g are supported by a compact set $\Sigma \subset \mathbb{R}^3$ (i.e., f and g are zero a.e. outside of Σ). Then the solution of (X.138) given by Theorem X.76a has the property that $u(\cdot, t)$ is supported by

$$\mathscr{C}(\Sigma, t) = \{x \in \mathbb{R} \mid \operatorname{dist}(x; \Sigma) \leq t\}$$

Proof First we prove the statement of the theorem for the *linear* equation

$$\begin{aligned} u_{tt} - \Delta u + m^2 u &= 0 \\ u(x, 0) &= f(x) \\ u_t(x, 0) &= g(x) \end{aligned} \tag{X.150}$$

Suppose first that f and g have support in S_R^0, the ball of radius R about zero. Then the solution of (X.150) is given by

$$u(t) = \cos(tB)f + B^{-1}\sin(tB)g$$

or, taking Fourier transforms,

$$\hat{u}(k, t) = \cos(t\sqrt{k^2 + m^2})\hat{f}(k) + (k^2 + m^2)^{-1/2}\sin(t\sqrt{k^2 + m^2})\hat{g}(k)$$

By the Paley–Wiener theorem (for distributions), $\hat{f}$ and $\hat{g}$ are entire analytic functions and there are constants C_i and integers N_i so that

$$\begin{aligned} |\hat{f}(k)| &\leq C_1(1 + |k|^2)^{N_1} e^{|\operatorname{Im} k|R} \\ |\hat{g}(k)| &\leq C_2(1 + |k|^2)^{N_2} e^{|\operatorname{Im} k|R} \end{aligned}$$

Further, since the roots drop out in the power series, $\cos(t\sqrt{k^2+m^2})$ and $(k^2+m^2)^{-1/2}\sin(t\sqrt{k^2+m^2})$ are also entire and satisfy

$$|\cos(t\sqrt{k^2+m^2})| \leq C_3 e^{|\operatorname{Im} k|t}$$
$$|(k^2+m^2)^{-1/2}\sin(t\sqrt{k^2+m^2})| \leq C_4 e^{|\operatorname{Im} k|t}$$

Thus $\hat{u}(k,t)$ is entire in k and there is a constant C and an integer N so that

$$|\hat{u}(k,t)| \leq C(1+|k|^2)^N e^{|\operatorname{Im} k|(R+t)}$$

By the converse part of the Paley–Wiener theorem $u(x,t)$ therefore has support in $S^0_{R+t} = \mathscr{C}(S^0_R, t)$. From the translation invariance of the equation it follows immediately that if f and g have their support in any sphere S, then $u(x,t)$ is supported by $\mathscr{C}(S,t)$. Finally, if f and g are supported by Σ, we can, given any $\varepsilon > 0$, find a finite number of spheres $S_1, \ldots, S_M$ so that $\Sigma \subset \bigcup_{i=1}^M S_i$ and $\bigcup_{i=1}^M S_i \subset \mathscr{C}(\Sigma, \varepsilon)$. Using again the fact that the solution depends linearly on the initial data, we easily conclude that the support of $u(x,t)$ is contained in $\bigcup_{i=1}^M \mathscr{C}(S_i,t)$ which is contained in $\mathscr{C}(\Sigma, t+\varepsilon)$. Since ε was arbitrary, $u(x,t)$ is supported by $\mathscr{C}(\Sigma,t)$.

We turn now to the nonlinear problem. Suppose that in the proof of Theorem X.72, we had chosen $\tilde{X}_{T,\varepsilon,\varphi_0} = \{\varphi(\cdot) \in X_{T,\varepsilon,\varphi_0} | \operatorname{supp}\varphi(t) \subset \mathscr{C}(\Sigma,t)\}$ instead of $X_{T,\varepsilon,\varphi_0}$. Then all the estimates work as before so we need only check that

$$(S\varphi)(t) = e^{-iAt}\varphi_0 + \int_0^t e^{-iA(t-s)}J(\varphi(s))\,ds$$

takes $\tilde{X}_{T,\varepsilon,\varphi_0}$ into itself (as far as the support property is concerned). By the result for the linear equation proven above, $e^{-iAt}\varphi_0$ has support in $\mathscr{C}(\Sigma,t)$. Further, if $\operatorname{supp}\varphi(s) \subset \mathscr{C}(\Sigma,s)$, then

$$\operatorname{supp} J(\varphi(s)) = \operatorname{supp}\langle 0, -\lambda|u(s)|^2u(s)\rangle$$
$$\subset \operatorname{supp}\varphi(s) \subset \mathscr{C}(\Sigma,s)$$

so by the linear result

$$\operatorname{supp}\{e^{-iA(t-s)}J(\varphi(s))\} \subset \mathscr{C}(\Sigma, s+(t-s)) = \mathscr{C}(\Sigma,t)$$

Thus $\int_0^t e^{-iA(t-s)}J(\varphi(s))\,ds$ is the integral of an $L^2(\mathscr{C}(\Sigma,t))$-valued function and so it too has support in $\mathscr{C}(\Sigma,t)$. Thus, S takes $\tilde{X}_{T,\varepsilon,\varphi_0}$ into itself so the unique fixed point $\varphi(t) = \langle u(x,t), u_t(x,t)\rangle$ which is our solution also has support in $\mathscr{C}(\Sigma,t)$ for each t. ∎

We conclude the section by showing that global existence does not hold in a large class of examples.

Example By applying the theorems of this section, one can easily prove local existence, uniqueness, and smoothness of solutions of the equation on $\mathbb{R}^2$:

$$\begin{aligned} u_{tt} - u_{xx} &= u^n \\ u(x, 0) &= u_0(x) \\ u_t(x, 0) &= v_0(x) \end{aligned} \tag{X.151}$$

where $x \in \mathbb{R}$ and $n > 1$. Further, if u_0 and v_0 are real-valued, then u is real-valued and, by the same argument as above, if u_0 and v_0 have compact support, then so will u for each t. So let u be a local solution of (X.151) where u_0 and v_0 are in $C_0^\infty(\mathbb{R})$. We will show that if u_0 and v_0 are chosen correctly, then

$$F(t) \equiv \int_{\mathbb{R}} u(x, t)^2 \, dx$$

goes to infinity in finite time. Suppose that we can find an $\alpha > 0$ and initial data u_0 and v_0 so that

$$\begin{aligned} &\text{(A)} \quad (F(t)^{-\alpha})'' \leq 0 \qquad \text{for all } t \geq 0 \\ &\text{(B)} \quad (F(t)^{-\alpha})' < 0 \qquad \text{at } t = 0 \end{aligned}$$

Then $F(t)^{-\alpha}$ will go to zero in finite time; see Figure X.8. Condition (B) is automatically satisfied by choosing u_0 and v_0 to have the same sign on $(-\infty, \infty)$ since

$$(F(0)^{-\alpha})' = -\alpha F(0)^{-1-\alpha} F'(0) = -2\alpha F(0)^{-1-\alpha} \int u_0 v_0 \, dx$$

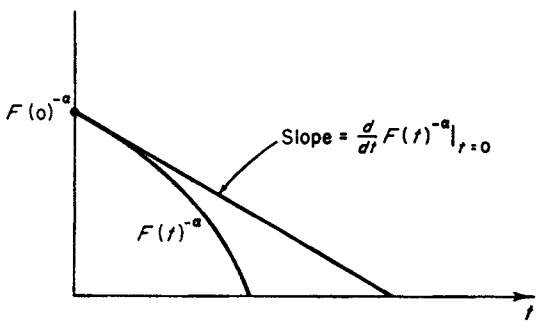


FIGURE X.8 The graph of $F(t)^{-\alpha}$.

so it remains to arrange for (A) to hold. Since $F(t) \geq 0$ this is the same as showing that $Q(t) \geq 0$ where

$$Q(t) \equiv (-\alpha)^{-1} F^{\alpha+2}(F^{-\alpha})'' = F''F - (\alpha+1)(F')^2$$

But,

$$F'(t) = 2\int uu_t\,dx$$

$$F''(t) = 2\int (uu_{tt} + u_t^2)\,dx$$

$$= 4(\alpha+1)\int u_t^2\,dx + 2\int (uu_{tt} - (2\alpha+1)u_t^2)\,dx$$

so,

$$Q(t) = 4(\alpha+1)\left\{\left(\int u^2\,dx\right)\left(\int u_t^2\,dx\right) - \left(\int uu_t\,dx\right)^2\right\}$$

$$+ 2F(t)\left\{\int uu_{tt}\,dx - \int (2\alpha+1)u_t^2\,dx\right\}$$

The first term on the right is positive by the Schwarz inequality, so we need only arrange that $H(t) \geq 0$ where

$$H(t) \equiv \int uu_{tt}\,dx - (2\alpha+1)\int u_t^2\,dx$$

$$= \int u^{n+1}\,dx + \int uu_{xx}\,dx - (2\alpha+1)\int u_t^2\,dx$$

$$= \int u^{n+1}\,dx - \int u_x^2\,dx - (2\alpha+1)\int u_t^2\,dx$$

The conserved energy for (X.151) is

$$E(t) = \frac{1}{2}\int (u_x^2 + u_t^2)\,dx - \frac{1}{n+1}\int u^{n+1}\,dx$$

That is, $E(t)$ is independent of t. Thus, if we choose α so that $2(2\alpha+1) = n+1$, we have

$$H(t) = -(n+1)E(t) + 2\alpha\int u_x^2\,dx$$

$$= -(n+1)E(0) + 2\alpha\int u_x^2\,dx \qquad \text{(X.152)}$$

Thus, if $E(0) < 0$, then H is always strictly positive since $\alpha = \frac{1}{4}(n-1) \geq 0$. Now, choosing $u_0 \geq 0$, $v_0 \geq 0$ so that (B) is satisfied, we scale u_0 by multiplying by a positive constant until $E(0) < 0$ (this will eventually happen since $n + 1 > 2$). For any such initial data, $F(t)$ goes to infinity in finite time.

If we consider instead the differential equation

$$u_{tt} - u_{xx} = -u^n$$

then $H(t)$ again satisfies (X.152), but now the conserved energy is

$$E(t) = \frac{1}{2}\int (u_x^2 + u_t^2)\, dx + \frac{1}{n+1}\int u^{n+1}\, dx$$

If n is even then by choosing $u_0(x) \leq 0$, $v_0(x) \leq 0$ (thus satisfying (B)) with u_0 sufficiently large we can obtain $E(0) \leq 0$ and thus the solution blows up in finite time. If, on the other hand, n is odd, then $E(t)$ is always greater than or equal to zero so the above argument does not work. This is not surprising since the $-u^3$ case is just the one-dimensional mass zero analogue of (X.138) where we have proven global existence.

X.14 The Hilbert space approach to classical mechanics

In this final section on the existence of dynamics, we want to briefly describe the L^2 approach to classical mechanics, its comparison with quantum theory and its limitations. Throughout, we will deal with systems whose phase space is $\mathbb{R}^{6N}$ (or $\mathbb{R}^{6N}$ with some singularity sets removed) and leave the discussion of more general symplectic manifolds to the Notes.

Let us begin with the formal elements of the theory. $\mathbb{R}^{6N}$ has a distinguished coordinate system p_i, q_i $(i = 1, \ldots, 3N)$ and a point in this **phase space** moves according to the equations of motion

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}; \qquad \dot{q}_i = \frac{\partial H}{\partial p_i} \tag{X.153}$$

where H is the energy function. In particular, a conservative Newtonian system

$$m_i \ddot{q}_i(t) = F_i(q_1, \ldots, q_{3N})$$

with

$$F_i(q) = -\frac{\partial V}{\partial q_i}$$

is of the form (X.153) if $H = \sum_{i=1}^{3N} (2m_i)^{-1} p_i^2 + V$.

(X.153) is, in general, a nonlinear ordinary differential equation in a finite-dimensional vector space. There is a standard method for rewriting such a system as a *linear* equation on an infinite-dimensional space. Namely, we transfer the action from points to functions. Let $\omega(q_0, p_0, t) = \langle q(t), p(t)\rangle$ where $\langle q(t), p(t)\rangle$ is the solution of (X.153) with initial data $q(0) = q_0$, $p(0) = p_0$. ω is a map from $\mathbb{R}^{6N+1}$ to $\mathbb{R}^{6N}$. Let

$$(U_t f)(q, p) = f(\omega(q, p; t)) \tag{X.154}$$

where f is a complex valued function on $\mathbb{R}^{6N}$. Then $U_t U_s = U_{t+s}$. We can formally compute the infinitesimal generator $i\, dU_t/dt$ by

$$\left.\frac{d(U_t f)}{dt}\right|_{t=0} = \sum_{i=1}^{3N} \frac{\partial f}{\partial q_i}\dot{q}_i + \frac{\partial f}{\partial p_i}\dot{p}_i$$
$$= \{f, H\} \tag{X.155}$$

by (X.153) where

$$\{f, g\} = \sum_{i=1}^{3N} \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}\right)$$

is the Poisson bracket. Obviously,

$$\{f, g\} = -\{g, f\} \tag{X.156}$$

and an integration by parts proves that

$$\int h\{f, g\}\, dp^{3N}\, dq^{3N} = \int \{h, f\}g\, d^{3N}p\, d^{3N}q \tag{X.157}$$

if $f, g, h \in C_0^\infty(\mathbb{R}^{6N})$.

These formal preliminaries suggest the following definition:

Definition Given any locally L^1 function $H(p, q)$ on $\mathbb{R}^{6N}$, we define the **Liouville form**, a quadratic form on $L^2(\mathbb{R}^{6N}, d^{3N}p\, d^{3N}q)$, with form domain $Q(\ell) = C_0^\infty(\mathbb{R}^{6N})$ by

$$\ell(f, g) = \int \{\bar{f}, g\}H\, d^{3N}p\, d^{3N}q \tag{X.158}$$

If H is a C^1 function, we define the **Liouville operator** on $C_0^\infty(\mathbb{R}^{6N})$ by

$$Lf = \{f, H\} \tag{X.159}$$

Using (X.156) and (X.157), it is easy (Problem 78) to prove:

Proposition

(a) The Liouville form is skew-symmetric, i.e.,

$$\ell(f, g) = -\overline{\ell(g, f)} \tag{X.160}$$

(b) If H is C^1 and $f, g \in D(L)$, then

$$(f, Lg) = \ell(f, g)$$

(c) $-iL$ is a symmetric operator.

If we know *global* existence and uniqueness of solutions of the classical ordinary differential equation (X.153), we can say more:

Theorem X.78 Let H be a C^1 function. Suppose that for each q_0, p_0, there is a unique C^1 function $\omega(q_0, p_0; t)$ from $\mathbb{R}$ to $\mathbb{R}^{6N}$ obeying (X.153) with initial condition $\omega(q_0, p_0; 0) = \langle q_0, p_0 \rangle$. Suppose that ω: $\mathbb{R}^{6N+1} \to \mathbb{R}^{6N}$ is a C^1 function. Then U_t is a unitary one-parameter group whose infinitesimal generator is $-i\bar{L}$. Moreover, $-iL$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{6N})$.

That U_t is unitary is known as **Liouville's theorem**.

Proof Let $D = C_0^1(\mathbb{R}^{6N})$, the C^1 functions of compact support. By an approximation of the identity argument (see the discussion in Section VIII.1), it is easy to see that $D \subset D(\bar{L})$ and that $\bar{L}f = \{f, H\}$ for any $f \in D$. Thus $\bar{L}$ is skew-symmetric on D. Now, since ω is C^1 by hypothesis, $U_t f$ is C^1 for each fixed t. Since $\omega(\cdot, \cdot; t)$ is a one-parameter group of maps of $\mathbb{R}^6$ to $\mathbb{R}^6$, $\{\langle p, q \rangle | \omega(p, q; t) \in \operatorname{supp} f\} = \{\omega(p, q; -t) | \langle p, q \rangle \in \operatorname{supp} f\}$ is compact if $f \in D$ as the continuous image of a compact set. Thus U_t defined as a map on D is a one-parameter group of operators from D to D. Moreover, for any f in D,

$$\frac{d}{dt} U_t f \Big|_{t=0} = \{f, H\} = \bar{L}f \tag{X.161}$$

To see this note that

$$t^{-1}[U_t f(q, p) - f(q, p)] - \{f, H\}(q, p)$$
$$= \frac{f(\omega(p, q; t)) - f(\omega(p, q; 0))}{t} - \sum_i \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right)$$

goes to zero pointwise by the chain rule. Moreover, since f has compact support and both f and ω are uniformly Lipschitz on compact sets, we can

dominate $t^{-1}(U_t f - f)$ by an L^2 function. Thus, by the dominated convergence theorem,

$$\|t^{-1}(U(t)f - f) - \{f, H\}\|_2 \to 0$$

so we have (X.161).

It follows by the skew symmetry of L that $(d/dt)\|U_t f\|^2 = 0$ so that U_t is bounded on D and $\|U_t f\| = \|f\|$. Thus U_t extends to a unitary operator on $\mathscr{H} = L^2(\mathbb{R}^{6N})$. Since it is given by (X.154) on D and any $f \in \mathscr{H}$ can be approximated by $f_n \in D$ with $f_n \to f$ pointwise a.e., U_t is given by (X.154) on all of $\mathscr{H}$. Since $U_t f$ is continuous for $f \in C_0^1$, it is continuous on $\mathscr{H}$. Finally, by the invariance of D under U_t, (X.161), and Theorem VIII.11, $-i\bar{L}$ is essentially self-adjoint on D and $-i\bar{L}$ is the infinitesimal generator of U_t. ∎

Unfortunately, it is usually not easy to prove that the classical equations of motion have global solutions, although if V is smooth and goes to plus infinity as $|x| \to \infty$, it is clear that solution curves stay bounded so that global solutions exist. We will presently see how to prove global existence for smooth V's which do not behave too badly at infinity. However, for many V's of interest, there are singularities at finite q, and, in fact, the equations of motion break down at "collisions." The natural thing to demand in such a situation is global existence for almost all initial conditions but even this has not been done for purely Coulomb forces if $N \geq 4$. Failing this, the next thing one might try is to prove that $-iL$ is essentially self-adjoint on some suitable set, like $C_0^\infty(M)$ where M is a dense set obtained by removing singular points from $\mathbb{R}^n$. This also remains open!

It is interesting to ask why self-adjointness results are so much easier in quantum mechanics than in classical mechanics. The reasons are several; we begin with the principal one.

(1) In the usual case, where $H = p^2 + V(q)$, $-iL$ is *never* bounded from below (or above). For let

$$(\theta f)(p, q) = f(-p, q)$$

Then

$$\theta L \theta^{-1} = -L$$

which is just an expression of the fact that $\omega(-p, q; t) = \omega(p, q; -t)$ ("time reversal invariance"), or $\theta(iL)\theta^{-1} = -iL$. Thus since $-iL$ is not bounded, it cannot be semibounded. If we define C by

$$Cf = \overline{\theta f}$$

then C is a complex conjugation with $C(-iL)C^{-1} = -iL$, so $-iL$ does have self-adjoint extensions by von Neumann's theorem (Theorem X.3).

This situation should be compared with quantum mechanics where $Cf = \bar{f}$ and $CHC^{-1} = H$, but where there is no real linear θ with $\theta H\theta^{-1} = -H$ forcing H to be unbounded both above and below.

Note that in both cases: $CqC^{-1} = q$; $CpC^{-1} = -p$.

(2) There is no dependence of p and q. Thus, if V is unbounded below, so is $H(p, q)$ while the quantum-mechanical energy operator may be bounded below on account of the uncertainty principle.

(3) Only V enters in the energy operator $-\Delta + V$ while derivatives of V enter in L. Thus singularities are made worse in L, so that, e.g. in the Coulomb case, $C_0^\infty \subset D(H_{\text{quantum}})$ but $C_0^\infty \not\subset D(L)$.

We close with an elementary existence theorem for (X.153) which will imply the skew-adjointness of L in some cases; the basic idea has already been used quite often (see the Appendix to Section X.1 and Section X.13) and is a classical analogue of Nelson's commutator theorem (see Example 4 in Section X.5).

Theorem X.79 Let V be a C^2 function on $\mathbb{R}^{3N}$ with $|\text{grad } V(q)| \leq C(q^2 + 1)^{1/2}$ for a suitable constant C. Let $H(p, q) = \sum_{i=1}^{3N} a_{ij} p_i p_j + V(q)$ where a is a strictly positive definite matrix. Then for any $\langle p_0, q_0 \rangle \in \mathbb{R}^{6N}$, there is a unique C^1 function from $\mathbb{R}$ to $\mathbb{R}^{6N}$, $\omega(p_0, q_0; t)$, satisfying (X.153) with initial conditions $\langle p_0, q_0 \rangle$. Moreover, $\omega(p_0, q_0, t)$ is a C^1 map of $\mathbb{R}^{6N+1}$ to $\mathbb{R}^{6N}$.

Proof Since V is C^2, the functions on the left-hand side of (X.153) are uniformly Lipschitz and uniformly bounded on compact subsets of $\mathbb{R}^{6N}$. Thus for any A, there is a $t(A) > 0$, so that $p_0^2 + q_0^2 + 1 \leq A$ implies that we can solve (X.153) for $|t| < t(A)$; see Section V.6. Now fix $\langle p_0, q_0 \rangle$. Let $(-T_0, T_1)$ be the maximum interval on which we can solve (X.153) with initial condition $\langle p_0, q_0 \rangle$. We will show that T_1 is ∞. For suppose not. For $0 \leq t < T_1$, let

$$N(t) = p(t)^2 + q(t)^2 + 1$$

Then

$$\begin{aligned}
\dot{N}(t) &= 2\dot{p}p + 2\dot{q}q \\
&\leq 2|p(t)||\text{grad } V(q(t))| + 2\|a\||p(t)||q(t)| \\
&\leq 2(C + \|a\|)(q^2(t) + 1)^{1/2}|p(t)| \\
&\leq (C + \|a\|)N(t)
\end{aligned}$$

Thus $N(t) \leq N(0)\exp[(C + \|a\|)t]$ for all $t > 0$. Let t_0 be the $t(A)$ for $A = N(0)\exp[(C + \|a\|)T_1]$. Choose $t \in (T_1 - t_0, T_1)$. Then we can solve (X.153) with initial condition $\langle p(t), q(t)\rangle$. By piecing this solution onto the supposed maximal solution, we obtain a solution in $(-T_0, t + t_0)$ contradicting maximality. Thus $T_1 = \infty$ and similarly $T_0 = \infty$.

By the method of Section X.13, ω is C^1 in the region obtained by one application of the contraction mapping principle. By the above argument, any t can be reached by finitely many applications of the contraction mapping principle (with successively larger starting times). ∎

Corollary Under the hypotheses of Theorem X.79, the Liouville operator L is essentially skew adjoint on $C_0^\infty(\mathbb{R}^6)$, i.e. $L^{**} = -L^*$.

NOTES

Section X.1 The main theorem of this section (Theorem X.2) was proven by J. von Neumann in "Allgemeine Eigenwerttheorie Hermitescher Funktionaloperatoren," *Math. Ann.* **102** (1929–1930) 49–131. The proof that we give is due to N. Dunford and J. Schwartz, *Linear Operators*, Vol. II, Wiley (Interscience), New York, 1963, who remark that their proof has many elements in common with the approach in J. Calkin, "Abstract symmetric boundary conditions," *Trans. Amer. Math. Soc.* **45** (1939) 369–442. The original approach of von Neumann makes extensive use of the *Cayley transform* of a symmetric operator A; this is formally defined by $V = (A - i)(A + i)^{-1}$. Some aspects of the proof become more transparent in the Cayley transform language, but the connection with boundary value problems is then not so clear. The main elements of the Cayley transform proof are: (i) V is defined as a map from $\overline{\text{Ran}(A + i)}$ to $\overline{\text{Ran}(A - i)}$ and can be shown to be a partial isometry, (ii) the deficiency indices of A are precisely the codimensions of the initial and final subspaces for V, (iii) closed symmetric extensions of A are in a one-to-one correspondence with extensions of V which are partial isometries. The self-adjoint extensions are in a one–one correspondence with unitary extensions of V. Unitary extensions of V are clearly characterized by an arbitrary unitary map from $D(V)^\perp$ to $\text{Ran}(V)^\perp$. One thereby obtains the fact that self-adjoint extensions of A exist only if $D(V) = \overline{\text{Ran}(A + i)}$ and $\text{Ran}(V) = \overline{\text{Ran}(A - i)}$ have equal codimension n, and the fact that the extensions are naturally parametrized by unitary maps from one n-dimensional space to another. For additional discussion of the extension theory from this Cayley transform point of view, see N. Akhiezer and I. Glazman, *Theory of Linear Operators in Hilbert Space*, Vol. II, Ungar, New York, 1963. There is further discussion of the "physical importance" of self-adjointness in A. S. Wightman, "Introduction to some aspects of the relativistic dynamics of quantized fields," *High Energy Electromagnetic Interactions and Field Theory* (M. Levy, ed.), Gordon and Breach, New York, 1967. For references for the moment problem, see the notes to Section X.6.

There is an alternative proof of Theorem X.3 which is essentially due to A. Galindo, "On the existence of J-self-adjoint extensions of J-symmetric operators with adjoint," *Comm. Pure Appl. Math.* **15** (1962), 423–425. We will sketch the proof which avoids the theory of self-adjoint

extensions (at the cost of using Zorn's lemma). Let A satisfy the hypotheses of Theorem X.3. Then, by Zorn's lemma, A has an extension B which satisfies the following three properties:

(i) $CB = BC$
(ii) $B \subset B^*$
(iii) B is maximal with respect to conditions (i) and (ii).

Suppose that $B \neq B^*$. Then we can find a nonzero $\langle \varphi, \psi \rangle \in \mathscr{H} \oplus \mathscr{H}$, so that

(iv) $\langle \varphi, \psi \rangle \in \Gamma(B^*) \cap \Gamma(B)^\perp$

Since $C \oplus C$ leaves both $\Gamma(B)$ and $\Gamma(B^*)$ invariant (by (i)), $\langle (I + C)\varphi, (I + C)\psi \rangle$ and $\langle i(I - C)\varphi, i(I - C)\psi \rangle$ are both in $\Gamma(B^*) \cap \Gamma(B)^\perp$ and at least one of them is nonzero. We can thus suppose that

(v) $\langle C\varphi, C\psi \rangle = \langle \varphi, \psi \rangle$

Let $\tilde{\Gamma} = \Gamma(B) \oplus \{\alpha \langle \varphi, \psi \rangle \mid \alpha \in \mathbb{C}\}$. Since $\tilde{\Gamma} \subset \Gamma(B^*)$, $\tilde{\Gamma}$ is the graph of an operator $\tilde{B}$. Because $C \oplus C$ leaves $\tilde{\Gamma}$ pointwise invariant, $\tilde{B}$ obeys (i). Moreover, since $\langle \varphi, \psi \rangle \in \Gamma(B)^\perp$, we have that for any $\eta \in D(B)$

$$(\varphi + \eta, \tilde{B}(\varphi + \eta)) = (\varphi, \psi) + (\eta, B\eta)$$

By (v), (φ, ψ) is real and, by (ii), $(\eta, B\eta)$ is real so $\tilde{B}$ is symmetric. Since this contradicts (iii), we conclude that $B = B^*$ and A has self-adjoint extensions.

Incidentally, the above proof shows that under the hypotheses of Theorem X.3, A has self-adjoint extensions commuting with C, a fact which also follows from a detailed analysis of the extensions of A. The existence of such extensions is important because it implies that *on a real Hilbert space every symmetric operator has self-adjoint extensions.* For $\mathscr{H} = \mathscr{H}_{\mathbb{R}} \oplus \mathscr{H}_{\mathbb{R}}$ can be viewed as a complex Hilbert space with $i\langle \varphi, \psi \rangle = \langle -\psi, \varphi \rangle$. Letting $C\langle \varphi, \psi \rangle = \langle \varphi, -\psi \rangle$, we see that every complex linear operator on $\mathscr{H}$ commuting with C is of the form $A \oplus A$ where $A: \mathscr{H}_{\mathbb{R}} \to \mathscr{H}_{\mathbb{R}}$. This fact, together with the strong form of Theorem X.3 yields the claimed fact about symmetric operators on real Hilbert spaces. For a further discussion, see Problem 81.

The discussion in the Appendix follows the general outline of unpublished lectures of E. Nelson. Further discussion of the self-adjointness of ordinary differential operators may be found in E. Coddington and N. Levinson, *Theory of Ordinary Differential Equations*, McGraw-Hill, New York, 1955 and in Chapter XIII of the book of Dunford and Schwartz mentioned above.

Extensive historical notes on the development of this self-adjointness theory may be found in Volume II of Dunford and Schwartz; we limit ourselves to mentioning that the limit point-limit circle theory (Theorems X.6 and X.7) is due to H. Weyl who introduced many of the ideas critical to the theory of extensions of unbounded operators many years before the development of the general theory of von Neumann. See H. Weyl, "Über gewöhnliche lineare Differentialgleichungen mit singulären Stellen und ihre Eigenfunktionen," *Nachr. Akad. Wiss. Göttingen Math.-Phys. Kl. II* (1909), 37–63, and (1910), 442–467; "Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen," *Math. Ann.* 68 (1910), 220–269. These papers can also be found in *Gesammelte Abhandlungen*, Vol. I, Springer-Verlag, Berlin, 1968.

The limit point-limit circle terminology arose from the idea of considering the self-adjointness problem for $-d^2/dx^2 + V(x)$ on (a, ∞) as a limit of problems on the interval (a, b) as $b \to \infty$. Let φ and ψ be the solutions of $-\varphi''(x) + V(x)\varphi(x) = i\varphi(x)$ on (a, ∞)

obeying $\varphi(a) = \psi'(a) = 0$, $-\varphi'(a) = \psi(a) = 1$. For fixed b, the set of $z \in \mathbb{C}$ for which $\eta = \varphi + z\psi$ obeys $(\cos\alpha)\eta(b) + (\sin\alpha)\eta'(b) = 0$ for some $\alpha \in [0, 2\pi)$ form a circle C_b. As $b \to \infty$, this circle either converges to a limiting circle or shrinks to a limiting point. In the former case, both solutions of $-\varphi''(x) + V(x)\varphi(x) = i\varphi(x)$ are L^2 near ∞; in the latter case, only one. This approach is further discussed in Coddington and Levinson.

Theorem X.8 appeared in N. Levinson, "Criteria for the limit-point case for second order linear differential operators," *Časopsis Pěst. Math. Fys.* **74** (1949) 17–20. We note that Theorem X.7 has an analogue for more general intervals than $[0, \infty)$; namely, if $V(x)$ is continuous on (a, b) with $-\infty \leq a < b \leq \infty$, then $-d^2/dx^2 + V(x)$ is in the limit point case at both a and b if and only if $-d^2/dx^2 + V(x)$ is essentially self-adjoint on $C_0^\infty(a, b)$. In particular, one can use Theorem X.8 to provide another proof of Problem 24 in the one-dimensional case. Theorem X.9 is due to A. Wintner in "On the Normalization of Characteristic Differentials in Continuous Spectra," *Phys. Rev.* **72** (1947) 516–517, and "The Schwartzian derivative and the approximation method of Brillouin," *Quart. Appl. Math.* **16** (1958), 82–86. A proof of Wintner's criterion and a variety of alternative criteria can be found in Dunford and Schwartz, Vol. II. The limit point case of Theorem X.10 is due to K. Friedrichs, "Über die ausgezeichnete Randbedingung in der Spektraltheorie der halbbeschränkten gewöhnlichen Differentialoperatoren zweiter ordnung," *Math. Ann.* **112** (1935/36), 1–23, and the limit circle part is due to D. Sears, "On the solutions of a linear second order differential equation which are of integrable square," *J. London Math. Soc.* **24** (1949), 207–215. Our proof is related to a general method of H. Kurss, "A limit-point criterion for non-oscillatory Sturm–Liouville differential operators," *Proc. Amer. Math. Soc.* **18** (1967), 445–449 (see Problem 8).

The first examples of potentials which are classically incomplete but quantum-mechanically complete were given in the 1949 Sears paper quoted above. The examples which we use are taken from J. Rauch and M. Reed, "Two examples illustrating the differences between classical and quantum mechanics," *Comm. Math. Phys.* **29** (1973), 105–111, and are based on suggestions of E. Nelson. H. Kalf has kindly sent to the authors his detailed analysis of Sears' example. Let V_{ab} be the potential on $(0, \infty)$ given by

$$V_{ab}(x) = \frac{2}{x^2} - 9x^4(a - 2b\cos(2x^3))$$

where a and b are in $(0, \infty)$. Then $-\varphi'' + V_{ab}\varphi = 0$ is the Mathieu equation whose general solution is

$$\frac{1}{x}\left(c_1 e^{\mu x^3}\varphi_{ab}(x^3) + c_2 e^{-\mu x^3}\varphi_{ab}(-x^3)\right)$$

where the exponent μ depends on a and b and $\varphi_{ab}(x)$ is a C^∞ function of period π unless $\langle a, b\rangle$ corresponds to a point on one of the curves in Figure X.9. The exponent μ is purely imaginary for $\langle a, b\rangle$ in the white regions of the figure and real for $\langle a, b\rangle$ in the shaded regions. V_{ab} is clearly both quantum-mechanically and classically complete at zero. At infinity, V_{ab} is quantum-mechanically complete if $\langle a, b\rangle$ falls in the shaded region since in that case μ is real so one solution is not in L^2 near infinity. However, if $\langle a, b\rangle$ is in the white region, then both solutions are in L^2 near infinity so V_{ab} is quantum-mechanically incomplete. Classically, if $2b < a$, then $V_{ab}(x) \leq -dx^4$ near infinity so a classical particle can escape to infinity in finite time, that is, V_{ab} is classically incomplete. On the other hand, if $2b > a$, then the peaks in the potential grow higher and higher so V is classically complete. For information about Mathieu functions, consult N. McLachlan, *Theory and Applications of Mathieu functions*, Oxford Univ. Press, London and New York, 1947, pp. 40, 98, or

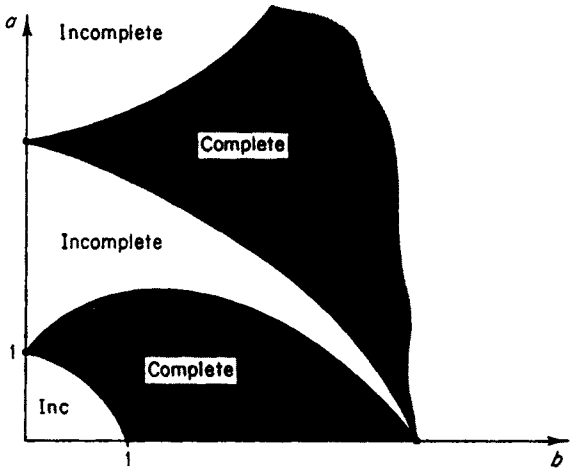


FIGURE X.9 Quantum-mechanical completeness for V_{ab}.

J. Meixner and F. Schäfke, *Mathieusche Funktionen und Sphäroidfunktionen*, Springer-Verlag, Berlin, 1954, p. 132.

Many of the criteria of essential self-adjointness of ordinary differential operators which can be derived from the Weyl theory can be generalized to partial differential operators. There is an analogue of Proposition 2 which plays an important role in these generalizations; this analogue is a theorem of E. Weinholtz, "Bemerkungen über elliptische Differentialoperatoren," *Arch. der Math.* **10** (1959), 126–133, and N. Nilsson, "Essential self-adjointness and the spectral resolution of Hamiltonian operators," *Kungl. Fys. Sällsk. i Lund Förh* **29**, (1959). These techniques played a role in various multidimensional extensions of Theorem X.8 (see the Notes to Section X.5).

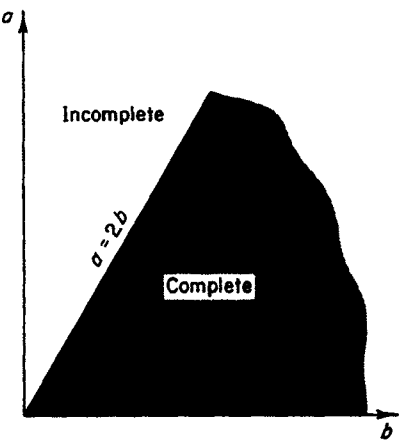


FIGURE X.10 Classical completeness for V_{ab}.

In many cases, the results obtainable by using the Weyl limit point–limit circle methods can be obtained more easily and in more generality by using the techniques of Sections X.4 and X.5.

The examples we discussed, where the classical and quantum mechanical conditions for completeness agree, required global conditions, i.e. conditions everywhere. But one would expect that a particle could be quantum mechanically trapped by a set of wide enough barriers, independent of what happens in between. A typical example in the one-dimensional case is the following theorem of R. S. Ismagilov, "Conditions for self-adjointness of differential operators of higher order," *Soviet Math.* **3** (1962), 279–283.

Theorem Let $V(x)$ be a continuous function $[0, \infty)$ and suppose there is a sequence of intervals (a_n, b_n), $b_n < a_{n+1}$, so that

(a) $V(x) \geq -(b_n - a_n)^{-2}$ for $x \in (a_n, b_n)$
(b) $\sum_n (b_n - a_n)^2 = \infty$

Then $-(d^2/dx^2) + V(x)$ is in the limit point case at infinity independent of the behavior of V outside of the intervals (a_n, b_n).

Notice that conditions (a) and (b) imply that the classical travel time across the union of the intervals (a_n, b_n) is infinite.

The first results of this general type requiring bounds only on intervals are due to P. Hartman, "The number of L^2-solutions of $x'' + q(t)x = 0$," *Amer. J. Math.* **43** (1951), 635–645. Other one-dimensional results can be found in M. S. P. Eastham, "On a limit-point method of Hartman," *Bull. London Math. Soc.* **4** (1972), 340–344, and N. P. Kupeov, "Conditions for non-self adjointness of a second order linear differential operator," *Soviet Math.* **2** (1961), 710–713. Theorems of this type applicable to noncentral potentials in many dimensions can be found in M. S. P. Eastham, W. D. Evans, and J. B. McLeod, "The Essential Self-Adjointness of Schrödinger-Type Operators," *Arch. Rational Mech. Anal.*, to appear. These authors also present examples of conditions in V in a tube $\Omega \times [0, \infty) \subset \mathbb{R}^n$ (Ω bounded and open in $\mathbb{R}^{n-1}$) so that if V obeys these conditions, then $-\Delta + V$ is not essentially self-adjoint on C_0^∞ independent of the behavior of V outside the tube. Intuitively in this case, the particle travels to infinity in the tube in finite time.

For a discussion of the Laplace–Beltrami operator used in Example 6, consult C. Müller, "Spherical Harmonics," Springer-Verlag *Lecture Notes in Mathematics* **17** (1966). In two dimensions, $B = d^2/d\theta^2$, $k_\ell = -\ell^2$, and there are two eigenfunctions corresponding to each $\ell > 0$, namely $e^{\pm i\ell\theta}$ and just the constant function corresponding to $\ell = 0$. The self-adjointness statement follows from the fact that $\{e^{i\ell\theta}\}_{\ell=-\infty}^{\infty}$ form a basis for $L^2(0, 2\pi)$. In three dimensions,

$$(Bg)(\theta, \phi) = (\sin\theta)^{-1}\left[\frac{\partial}{\partial\theta}(\sin\theta)\frac{\partial g}{\partial\theta} + \frac{\partial}{\partial\phi}(\sin\theta)^{-1}\frac{\partial g}{\partial\phi}\right]$$

where θ and ϕ are the usual angular variables in spherical coordinates. In this case $k_\ell = -\ell(\ell+1)$ and the corresponding eigenspace has dimension $2\ell + 1$. In s dimensions, $k_\ell = -\ell(\ell + s - 2)$. There is a close connection between B and the representation theory of the group $SO(s)$. In particular, there is a connection between the completeness of the eigenfunctions of B and the Peter–Weyl theorem (see Chapter XIV).

Section X.2 Theorem X.12 is due to F. Rellich: "Störungstheorie der Spektralzerlegung, II," *Math. Ann.* **116** (1939) 555–570. A wide variety of applications and extensions of the Kato–Rellich theorem can be found in the book, T. Kato, *Perturbation Theory for Linear*

Operators, Springer, New York, 1966. In particular, Theorem X.13 and the special case of Theorem X.14 where (X.21a) is replaced with the stronger condition (X.21b) (equivalently (X.21c)) appear in Kato's book. Theorem X.14 is due to R. Wüst, "Generalizations of Rellich's theorem on perturbations of (essentially) self-adjoint operators," *Math. Z.* **119** (1971) 276–280; for additional discussion, see R. Wüst, "Holomorphic operator families and stability of self-adjointness," *Math. Z.* **125** (1972), 349–358.

Kato's application of Rellich's theorem to atomic Hamiltonians appeared in T. Kato, "Fundamental properties of Hamiltonian operators of Schrödinger type," *Trans. Amer. Math. Soc.* **70** (1951), 195–211. This paper was a turning point in mathematical physics for two reasons. Firstly, the proof of self-adjointness was a necessary preliminary to the problems of spectral analysis and scattering theory for these operators, problems which have occupied mathematical physicists ever since. Secondly, the paper focused attention on specific systems rather than foundational questions.

The KLMN theorem in various forms is due to T. Kato, "Quadratic forms in Hilbert space and asymptotic perturbation series," Technical report No. 7, Univ. of Calif. (1955); J. Lions, *Équations Différentielles Opérationelles et Problèmes aux Limites*, Springer-Verlag, Berlin, 1961, Chapter II, Section 1; and P. Lax and A. Milgram, "Parabolic equations," in *Contributions to the theory of partial differential equations*, *Ann. Math. Study* **33**, Princeton, New Jersey, 1954. The interpretation of the theorem in terms of scales of spaces was first emphasized by E. Nelson, "Interaction of nonrelativistic particles with a quantized scalar field," *J. Math. Phys.* **5** (1964) 1190–1197.

Written in terms of operator inequalities, Theorem X.18 is slightly weaker than the statement "If $0 \leq A^2 \leq B^2$, then $0 \leq A \leq B$" which is known as the monotonicity of the square root. This is a special case of the following theorem of K. Löwner, "Über monotone Matrixfunktionen," *Math. Z.* **38** (1934), 177–216:

Theorem A necessary and sufficient condition for a continuous real-valued function f on $(0, \infty)$ to have the property that $f(A) \leq f(B)$ for all pairs of self-adjoint operators, A, B with $0 < A \leq B$ is that f be the restriction to $(0, \infty)$ of a function f analytic in $\mathbb{C}\backslash(-\infty, 0]$ with the property $(\operatorname{Im} f) \geq 0$ for all z with $\operatorname{Im} z > 0$.

The "physical" argument behind the expectation that quantum mechanics can be developed for potentials with $r^{-\alpha}$ singularities $0 < \alpha < 2$ is based on the following heuristics: First, the basic property required for a nonpathological physics is the semiboundedness of $H_0 + V$; secondly, if a wave function is concentrated in a region of size Δr about a negative $r^{-\alpha}$ singularity, then by the uncertainty principle, the expectation value of H_0 is on the order of $(\text{const})(\Delta p)^2 \approx (\text{const})(\Delta r)^{-2}$ while the expectation value of V is on the order of $(\text{const})(\Delta r)^{-\alpha}$. Since $cx^{-2} - dx^{-\alpha}$ $(c, d > 0)$ is semibounded only if $0 < \alpha \leq 2$, we expect reasonable physics to break down at $\alpha = 2$.

The inequality that we have dubbed the uncertainty principal lemma is classical; see for example H. Kalf and J. Walter, "Strongly singular potentials and essential self-adjointness of singular elliptic operators in $C_0^\infty(\mathbb{R}^n\backslash\{0\})$," *J. Functional Analysis* **10** (1972), 114–130, where historical remarks are given. That $r^{-2} < -c\Delta$ for some constant is a special case of a theorem of the same type as Theorem X.21: If $s > 3$ and $V \in L^{s/2}_w$, then V is Δ-form bounded with bound less than or equal to $c\|V\|_{s/2,w}$.

The development of much of the operator theory needed for the quantum mechanics of Hamiltonians with Rollnik potentials and in particular the proof of Theorem X.19 may be found in B. Simon, *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms*, Princeton Univ. Press, Princeton, New Jersey, 1971. The reader can also find there a summary of the discovery and rediscovery of the Rollnik condition by various authors.

The extension of Kato's theorem to n dimensions has been discussed by a variety of authors. Theorem X.20 appeared in F. Brownell, "A note on Kato's uniqueness criterion for Schrödinger operator selfadjoint extensions," *Pacific J. Math.* **9** (1959), 953–973; our proof of it is borrowed from an appendix of E. Nelson, "Feynman integrals and the Schrödinger equation," *J. Math. Phys.* **5** (1964) 332–343. A closely related discussion of n-dimensional potentials already appeared in F. Stummel, "Singuläre elliptische Differentialoperatoren in Hilbertschenräumen," *Math. Ann.* **132** (1956) 150–176. Stummel's results were not stated in terms of L^p spaces but in terms of conditions of the form:

$$\int_{|x-y|\leq 1} |x-y|^{-s+4-\alpha} |V(y)|^2 \, dy \leq C \qquad \text{for all } x$$

for some $\alpha > 0$. In much of the literature on Schrödinger operators, these "Stummel conditions" and the related "Stummel spaces" Q_α are used.

A direct proof of the extension of Theorem X.20 to the boundary case $p = s/2$ ($s \geq 5$) was given in W. Faris, "The product formula for semi-groups defined by Friedrichs extensions," *Pacific J. Math.* **22** (1967) 47–70. His proof uses the Sobolev embedding theorem which is in turn based on the classical Sobolev inequality discussed in Section IX.4. Strichartz' theorem in a slightly different form appears in R. Strichartz, "Multipliers on Fractional Sobolev spaces," *J. Math. Mech.* **16** (1967), 1031–1060. The applicability of this theorem to Schrödinger operators is an unpublished remark of Nelson.

That r^{-2} is a Δ-bounded perturbation on $\mathbb{R}^s$ if $s \geq 5$ follows from an explicit operator estimate of classical form: if $u \in C_0^\infty(\mathbb{R}^s \backslash \{0\})$ and if $a \geq -\frac{1}{2}s(s-4)$, then

$$\int |\Delta u|^2 \, d^s x \geq -a \int \frac{|\nabla u|^2}{|x|^2} \, d^s x + \frac{(s-4)^2}{16} (s^2 + 4a) \int \frac{|u|^2}{|x|^4} \, d^s x$$

This inequality of Rellich's is proven in F. Rellich, *Perturbation theory of eigenvalue problems*, Gordon and Breach, New York, 1969; see also the paper of Schmincke quoted below.

Konrady's trick and its application to the field theory generalization of the anharmonic oscillator appear in J. Konrady, "Almost positive perturbations of positive self-adjoint operators," *Comm. Math. Phys.* **22** (1971), 295–299. At about the same time, the same method was independently discovered in U.-W. Schmincke, "Essential self-adjointness of a Schrödinger operator with strongly singular potential," *Math. Z.* **124** (1972), 47–50.

Section X.3 In his original paper on self-adjoint extensions (see the Notes to Section X.1), von Neumann proved that a semibounded operator has semibounded extensions whose lower bound is arbitrarily close to the bound of the original operator. He conjectured that extensions exist with the same lower bound. This fact, i.e. Theorem X.23, was proven by K. Friedrichs in "Spektraltheorie halbbeschränkter Operatoren," *Math. Ann.* **109** (1934), 465–487, and by M. Stone in *Linear Transformations in Hilbert Spaces and their Applications in Analysis*, Amer. Math. Soc. Colloquium Publication **15**, Providence, Rhode Island, 1932. For further discussion of when the Friedrichs extension is the unique extension with the same lower bound (Example 1), see E. T. Poulsen, "The minimax principle and uniqueness of the Friedrichs extension," *Proc. Amer. Math. Soc.* **21** (1969), 508–509. Theorem X.24 and the proposition preceding it are due to M. Krein, "The theory of self-adjoint extensions of semibounded Hermitean operators and its applications, I," *Mat. Sb.* **20** (1947), 431–495, and is further discussed in B. Simon, "The theory of semi-analytic vectors: a new proof of a theorem of Masson and McClary," *Indiana Univ. Math. J.* **20** (1971), 145–151.

Theorem X.25 was first proven in J. von Neumann, "Uber adjungierte Funktionaloperatoren," *Ann. Math.* **33** (1932), 249–310.

Section X.4 Kato's inequality is due to T. Kato, "Schrödinger Operators with Singular Potentials," *Israel J. Math.* **13** (1973), 135–148. Theorem X.28 and X.29 also appear there. Kato was motivated in part by B. Simon, "Essential self-adjointness of Schrödinger operators with positive potentials," *Math. Ann.* **201** (1973), 211–220. Simon had proven Theorem X.28 under the stronger hypothesis $V \geq 0$, $V \in L^2(\mathbb{R}^n, \exp(-ax^2)\,d^nx)$ for some a. Previous to Simon's work, it was a folk belief that V had to be in a local Stummel space (essentially that V be in L^p_{loc} for some $p > n/2$ if $n \geq 4$) if $-\Delta + V$ was to be essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Weaker versions of Theorem X.28 are quite old. In particular, that $-\Delta + V$ is essentially self-adjoint if $V \geq 0$ and $V \in C_0^\infty(\mathbb{R}^n)$ is a result of T. Carleman, "Sur la théorie mathématique de l'équation de Schrödinger," *Ark. Mat., Ast., Fys.* **24B**, No. 11 (1934). His result was independently rediscovered by A. Jaffe, "A $\lambda\varphi^4$ Cutoff Field Theory," Princeton Univ. thesis, Princeton, New Jersey, 1965. The extension to some classes of singular positive V was first accomplished by F. Stummel (see the Notes to Section X.2). Perhaps the strongest version of the result preceding Kato's paper appeared in H. Stetkaer-Hansen, "A generalization of a theorem of Wienholtz concerning essential self-adjointness of singular elliptic operators," *Math. Scand.* **19** (1966), 108–112 and J. Walter, "Note on a paper by Stetkaer-Hansen concerning essential self-adjointness of Schrödinger operators," *Math. Scand.* **25** (1969), 94–96, who proved a stronger result if $n \leq 3$ and a weaker theorem if $n \geq 4$.

Theorem X.30 appears in B. Simon, "Essential Self-Adjointness of Schrödinger-Operators with Singular Potentials: A Generalized Kalf–Walter–Schmincke Theorem," *Arch. Rational Mech. Anal.* **52** (1973), 44–48. A partially alternative proof can be found in H. Kalf and J. Walter, "Note on a paper of Simon on the essential self-adjointness of Schrödinger operators with singular potentials," *Arch. Rational Mech. Anal.* **52** (1973), 258–260. Simon's result generalizes results of H. Kalf and J. Walter, "Strongly singular potentials and essential self-adjointness of singular elliptic operators on $C_0^\infty(\mathbb{R}^n\backslash\{0\})$," *J. Functional Analysis* **10** (1972), 114–130, and of U.-W. Schmincke, "Essential self-adjointness of a Schrödinger operator with strongly singular potential," *Math. Z.* **124** (1972), 47–50. The earliest results of the genre are due to K. Jörgens, "Wesentliche Selbstadjungiertheit singulärer elliptischer Differentialoperatoren zweiter Ordnung in $C_0^\infty(G)$," *Math. Scand.* **15** (1964), 5–17.

Theorem X.31 is due to W. Faris, "Essential self-adjointness of operators in ordered Hilbert space," *Comm. Math. Phys.* **30** (1973), 23–34. A slightly weaker theorem was proven earlier by E. B. Davies, "Properties of the Green's functions of some Schrödinger operators," *J. London Math. Soc.* **7** (2) (1973), 473–491.

The first comprehensive treatment of Schrödinger operators with magnetic fields appears in T. Ikebe and T. Kato, "Uniqueness of the self-adjoint extension of singular elliptic differential operators," *Arch. Rational Mech. Anal.* **9** (1962), 77–92. They proved a theorem like Theorem X.34 but with stronger conditions on V. Theorem X.34 is from Kato's *Israel Journal* article. Kato proved Theorem X.33 under the weaker condition that $u \in L^1_{\text{loc}}$. We have simplified the proof by noting that $u \in L^2_{\text{loc}}$ is sufficient in applications. This remark is critical for the proof of Theorem X.35 which can be found in B. Simon, "Schrödinger operators with singular magnetic vector potentials," *Math. Z.* **131** (1973), 361–370. Simon's paper is based on a strengthened version of the technical lemma for Theorem X.33. Results similar to Theorem X.35 may be found in M. Schechter, *Spectra of Partial Differential Operators*, North-Holland, Amsterdam, 1971. Previous to Simon's paper, the use of Coulomb gauge was advocated by K. Jörgens, "Uber das wesentliche Spektrum elliptischer Differentialoperatoren vom Schrödinger-Typ," Tech. report, Univ. Heidelberg, 1965, and "Zur Spektraltheorie der Schrödingeroperatoren," *Math. Z.* **96** (1967), 355–372.

Theorem X.32 is due to T. Kato, "A second look at the essential self-adjointness of the Schrödinger operators," to appear.

Earlier results describing the domain of the Friedrichs extension can be found in K. Friedrichs, "Spektraltheorie halbbeschränkter Operatoren und Anwendung auf die Spektralzerlegung von Differentialoperatoren, II," **109** (1933/34), 685–713 (corrections in *Math. Ann.* **110** (1934/35), 777–779), and "Uber die ausgezeichnete Randbedingung in der Spektraltheorie der halbbeschränkter gewöhnlichen Differentialoperatoren zweiter Ordnung," *Math. Ann.* **112** (1935/36), 1–23; H. Freudenthal, "Über die Friedrichysche Fortsetzung halbbeschränkter Hermitescher Operatoren," *Nederl. Akad. Wetensch. Proc. Ser.* **39** (1936), 832–833; F. Rellich, "Halbbeschränkte gewöhnliche Differentialoperatoren zweiter Ordnung," *Math. Ann.* **122** (1950/51), 343–368; H. Kalf, "On the characterization of the Friedrichs extension of ordinary or elliptic differential operators with a strongly singular potential," *J. Functional Analysis* **10** (1972), 230–250.

Section X.5 Nelson's commutator theorem appeared in E. Nelson, "Time-ordered operator products of sharp-time quadratic forms," *J. Functional Analysis* **11** (1972), 211–219. Earlier a similar theorem appeared in J. Glimm and A. Jaffe, "The $\lambda(\varphi^4)_2$ quantum field theory without cutoffs, IV: Perturbation of the Hamiltonian," *J. Math. Phys.* **13** (1972), 1568–1584. The Glimm-Jaffe theorem was weaker in that bounds on both the commutator and double commutator were needed. Both Nelson and Glimm-Jaffe intended the theorem for application to the self-adjointness of smeared quantum field operators by the scheme used in Example 3. Nelson's paper also contained Lemmas 1 and 2.

Both the Nelson paper and the Glimm–Jaffe paper have somewhat more complicated proofs than the one we use and both use the not-quite-standard techniques of mollifiers and graph limits respectively. The simple proof that we use, based on the fundamental criterion, was noted by W. Faris and R. Lavine, "Commutators and self-adjointness of Hamiltonian operators," *Comm. Math. Phys.* **35** (1974), 39–48. They also give a proof based on the intuition of Example 4 and applied the theory to Schrödinger operators (Theorem X.38 and its corollaries) and to Dirac operators.

An alternative proof and a slightly more general result appear in O. McBryan, "Local generators for the Lorentz group in the $P(\varphi)_2$ model," *Nuovo Cimento* **18A** (1973), 654–662.

In Stummel's 1956 paper (see the Notes to Section X.2), the Hamiltonian of the hydrogen atom in an asymptotically constant electric field is proven essentially self-adjoint. More general atoms in constant fields were first treated in the Ikebe–Kato paper (see the Notes to Section X.4). Earlier, operators of the form $-\Delta + V$ with V *continuous* and $V(x) \geq -cx^2 - d$ were proven essentially self-adjoint on C_0^∞ by N. Nilsson (see the Notes to Section X.2). These results were further generalized by B. Hellwig, "Ein Kriterium für die Selbstadjungiertheit elliptischer Differentialoperatoren in $\mathbb{R}^n$," *Math. Z.* **86** (1964), 255–262 and "A criterion for self-adjointness of singular elliptic differential operators," *J. Math. Anal. Appl.* **26** (1969), 279–291. In particular, these papers contain a multi-dimensional version of Theorem X.8.

The second Corollary to Theorem X.38 is proven by alternative methods in H. Kalf, "Self-adjointness for strongly singular potentials with a $-|x|^2$ fall-off at infinity," *Math. Z.* **133** (1973), 249–255.

For Dirac operators, there is no restriction on how quickly V can grow at infinity. P. Chernoff in "Essential Self-Adjointness of Powers of Generators of Hyperbolic Equations," *J. Func. Anal.* **12** (1973), 401–414, remarked that this is intuitively correct since the relativistic bound $|v| < c$ prevents finite travel time to infinity. For strong results on the self-adjointness of Dirac operators, the reader can consult W. D. Evans, "On the Unique Self-Adjoint Extension of the Dirac Operator and the Existence of the Green Matrix," *Proc. London Math. Soc.* **20** (3) (1970), 537–557, and U.-W. Schmincke, "Essential Self-Adjointness of Dirac Operators with Strongly Singular Potentials," *Math. Z.* **126** (1972), 71–81.

Section X.6 Analytic vectors first appeared in the context of group representations in the work of Harish-Chandra, "Representations of a semi-simple Lie group on a Banach space, I," *Trans. Amer. Math. Soc.* **75** (1953), 185–243, and P. Cartier and J. Dixmier, "Vecteurs analytiques dans les représentations de groupes de Lie," *Amer. J. Math.* **80** (1958), 131–145. Their use in the study of a single operator was emphasized and developed by E. Nelson in "Analytic Vectors," *Ann. Math.* **70** (1959), 572–615. Given a continuous unitary representation $U(\cdot)$ of a Lie group G on a Hilbert space $\mathscr{H}$, Gårding had previously shown how to construct a common dense invariant domain for the generators of one-parameter subgroups of $U(G)$, i.e., for the representation of the Lie algebra g of G. In his paper, Nelson showed how to construct a common, dense, invariant domain of essential self-adjointness for all the generators by finding a domain that contained a dense set of analytic vectors for all the generators. Nelson also proved that if a Lie algebra is represented by symmetric operators on a dense invariant domain, then, if the domain contains a dense set of analytic vectors, the representation of the Lie algebra arises by differentiating a unique representation of the corresponding Lie group. These results have been extended; see, for example, J. Simon, "On the integrability of representations of finite-dimensional real Lie algebras," *Comm. Math. Phys.* **28** (1972), 39–46.

The generalization of Nelson's result given in Theorem X.40 is due to A. Nussbaum, "A note on quasi-analytic vectors," *Studia Math.* **33** (1969), 305–310. The simple proof outlined in Problem 42 originally appeared in B. Simon, "The theory of semi-analytic vectors: a new proof of a theorem of Masson and McClary," *Indiana Univ. Math. J.* **20** (1971) 1145–1151.

Nussbaum's lemma appears in "Quasi-analytic vectors," *Ark. Mat.* **6** (1965) 179–191. Nussbaum also introduced a generalization of the notion of analytic vectors. A vector $\varphi \in C^\infty(A)$ is called **quasi-analytic** if

$$\sum_{n=0}^{\infty} \|A^n\varphi\|^{-1/n} = \infty$$

An analytic vector is quasi-analytic, but the converse is not necessarily true. Nussbaum proves that a closed symmetric operator whose domain contains a dense set of quasi-analytic vectors is self-adjoint. Nussbaum also proves (in his *Studia Math.* paper) that a semibounded closed symmetric operator with a dense set of vectors satisfying

$$\sum_{n=1}^{\infty} \|A^n\varphi\|^{-1/2n} = \infty$$

is self-adjoint. Such vectors are called **Stieltjes vectors**. This result was obtained independently by D. Masson and W. McClary, "Classes of C^∞-vectors and essential self-adjointness," *J. Functional Analysis* **10** (1972) 19–32. Both the Nussbaum and the Masson–McClary papers use techniques from the moment problem. Essentially, they turn around the argument in Examples 4 and 6 and use classical results on the moment problem to prove that certain vectors are vectors of uniqueness. A critical result linking the two notions is in Nussbaum's *Arkiv* paper: $\varphi \in C^\infty(A)$ is a vector of uniqueness if and only if the Hamburger moment problem for $a_n = (\varphi, A^n\varphi)$ has a unique solution. The relationship between self-adjointness and the moment problem goes back at least as far as Stone's classic *Linear Transformations in Hilbert Space and Their Applications to Analysis*, Amer. Math. Soc. Colloquium Publication XV, New York (1932). Two general references for the moment problem are: J. Shohat and J. D. Tamarkin, *The Problem of Moments*, Amer. Math. Soc., New York, 1943, and Ya. V. Vorobyev, *Method of Moments in Applied Mathematics*, Gordon and Breach, New York, 1965.

Section X.7 Fock space was introduced by V. Fock in his paper "Konfigurationsraum und zweite Quantelung," *Z. Phys.* **75** (1932), 622–647. The first proof of the self-adjointness of the fields on Fock space was given by J. Cook: "The mathematics of second quantization," *Trans. Amer. Math. Soc.* 74 (1953), 222–245. Cook proved directly that $\varphi(f) \pm i$ and $\pi(f) \pm i$ have dense ranges on F_0.

The abstract structure of free fields was extensively studied in the 1950's by K. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields*, Wiley (Interscience), 1953, and by I. Segal in a series of papers; see especially "Tensor Algebras over Hilbert spaces, I," *Trans. Amer. Math. Soc.* **81** (1956), 106–134, where Q space was introduced. This led Segal to study the connection between the free field and probability theory and, in particular, he found a connection between abstract Fock spaces and Wiener path integrals.

For a discussion of the Wightman axioms, see Section IX.8 and the notes to that section. Wick ordering was introduced in G.-C. Wick: "The Evaluation of the Collision Matrix," *Phys. Rev.* **80** (1950), 267–272. General results on Wick ordered free fields may be found in L. Gårding and A. Wightman: "Fields as operator-valued distributions in relativistic quantum field theory," *Ann. Phys.* **16** (1961), 158–176.

Wick also emphasized the combinatorial structure of the vacuum expectation values of the free field. In particular, one has the following formulas:

$$(\Omega_0, \varphi(x_1) \cdots \varphi(x_n)\Omega_0) = 0 \qquad \text{if } n \text{ is odd}$$

$$(\Omega_0, \varphi(x_1) \cdots \varphi(x_{2n})\Omega_0) = \sum_{\substack{i_1 < \cdots < i_n \\ i_k < j_k \\ i_1, \ldots, j_n \text{ distinct}}} (\Omega_0, \varphi(x_{i_1})\varphi(x_{j_1})\Omega_0) \cdots (\Omega_0, \varphi(x_{i_n})\varphi(x_{j_n})\Omega_0) \tag{X.162}$$

This complicated expression is a sum over all distinct ways of writing $\{1, \ldots, 2N\}$ as N pairs. (X.162) is one of a number of formulas that usually go under the name "Wick's theorem." Many of these formulas are well organized in a book by E. Caianiello, *Combinatorics and Renormalization in Quantum Field Theory*, Addison-Wesley, Reading, Massachusetts, 1973. (X.162) says that *for the free field* one can compute the Wightman distributions knowing only the two point function. There is a large class of models for which this is true: Let ρ be any polynomially bounded measure on $[0, \infty)$. Define

$$(\Omega_0, \varphi(x)\varphi(y)\Omega_0) = \int \Delta_+(x - y, m^2)\, d\rho(m^2)$$

and let the n-point distribution be given by (X.162). It can be shown that these distributions are the Wightman distributions of a unique quantum field theory satisfying the Wightman axioms. It is called the "generalized free field with spectral weight ρ." Like the free field, these theories are trivial in that the scattering matrix is the identity (when it exists). The generalized free field was introduced by W. Greenberg in "Generalized free fields and models of local field theory," *Ann. Phys.* **16** (1961), 158–176.

Number operator estimates of the kind found in Theorem X.44 were first used systematically by J. Glimm in "Yukawa coupling of quantum fields in two dimensions," *Comm. Math. Phys.* **5** (1967), 343–386. A thorough discussion of these estimates can be found in the lectures by J. Glimm and A. Jaffe "Some quantum field theory models" in *Statistical Mechanics and Quantum Field Theory* (Les Houches, 1970), ed. by C. deWitt and R. Stora, Gordon and Breach, New York, 1971.

We continue the study of the $(\varphi^4)_2$ model in Section X.9 and Chapter XIX where a detailed history will be given. L^p properties of the spatially cut-off interaction were first emphasized by E. Nelson, "A quartic interaction in two dimensions," in *Mathematical*

Theory of Elementary Particles (R. Goodman and I. Segal, eds.), MIT Press, Cambridge, Massachusetts, 1966, who discovered the fact that $e^{-tV} \in L^1$. A detailed proof can be found in the Glimm–Jaffe lectures quoted above. For properties of the $(\varphi^4)_3$ interaction see J. Glimm and A. Jaffe, "Positivity of the $(\phi^4)_3$-Hamiltonian," *Fortschr. Physik* **21** (1973), 327–376, and the references therein.

The idea that Euclidean invariance is deeply connected with questions of inequivalence of representations of the CCR—an idea which is basic to our proof of Theorem X.46—is part of a complex of ideas generally called "Haag's theorem" after the discoveries of R. Haag in "On Quantum Field Theories," *Danske Vid. Selsk. Mat.-Fys. Medd.* **29** 12 (1955). The use of translation invariance suggests that the inequivalence of representations for different masses is "at infinity." This is true in the following sense: Given any bounded region B in $\mathbb{R}^3$ and free fields $\{\varphi_{m_1}, \pi_{m_1}\}$, $\{\varphi_{m_2}, \pi_{m_2}\}$ on $\mathscr{H}_1$ and $\mathscr{H}_2$, there is a unitary map U_B: $\mathscr{H}_1 \to \mathscr{H}_2$ so that $U_B \varphi_{m_1}(f) U_B^{-1} = \varphi_{m_2}(f)$ and $U_B \pi_{m_1}(f) U_B^{-1} = \pi_{m_2}(f)$ if supp $f \subset B$. This "local equivalence" appears again in Chapter XIX, both in our study of the free field algebras and in our discussion of the "local Fock property" of the $(\varphi^4)_2$ model.

Our construction of Q space is basis dependent in that it depended on the choice $\{f_n\}_{n=1}^{\infty}$. What is independent of the choice of basis is the algebra of measurable sets (modulo sets of measure zero) and the measure on these sets. There are many other "realizations" of Q space where the "points" differ, but the algebra of measurable sets and the measure are the same.

L. Gårding and A. S. Wightman classified all the representations of the relations (X.95) in "Representations of the canonical commutation relations," *Proc. Nat. Acad. Sci. U.S.A.* **40** (1954), 622–626. It is possible that von Neumann knew of the existence of inequivalent representations as early as 1938 since one can use his theory of infinite tensor products ("On Infinite Tensor Products," *Compositio Math.* **6** (1939), 1–77) to construct easily uncountably many inequivalent representations: see L. Streit: "Test function spaces for direct product representations," *Comm. Math. Phys.* **4** (1967), 22–31. The self-adjointness of the canonical fields of (X.95) in arbitrary representations was proven by M. Reed, "A Gårding domain for quantum fields," *Comm. Math. Phys.* **14** (1969), 336–346. Reed showed that for any representation in the Gårding–Wightman classification, there is a Banach space B of test functions (B depends on the representation) so that $\varphi(f)$ and $\pi(f)$ are self-adjoint for $f \in B$.

A classification of representations of the CCR in continuous form (X.94) can be found in several places; see, e.g., I. M. Gel'fand and N. Vilenkin, *Generalized Functions IV*, Academic Press, New York, 1964, p. 370. Reed's theorem has been extended to the continuous CCR by G. Hergerfeldt, "Gårding domains and analytic vectors for quantum fields," *J. Math. Phys.* **13** (1972), 821–827. His theorem is quoted on page 232.

Section X.8 The study of semigroups of linear transformations has its origin in M. Stone's paper on unitary groups in Hilbert space: "Linear transformations in Hilbert space III," *Proc. Nat. Acad. Sci. U.S.A.* **16** (1930), 172–175. The Hille–Yosida theorem for the case of contraction semigroups (Theorem X.47a) was proven independently by E. Hille: *Functional analysis and semi-groups*, Amer. Math. Soc. Colloquium Publication, **31**, 1948, New York, and "On the generation of semi-groups and the theory of conjugate functions," *Kungl. Fys. Sälls. I Lund Förhand.* **21** (1952), 1–13, and by K. Yosida: "On the differentiability and representation of one-parameter semi-groups of linear operators," *J. Math. Soc. Japan* **1** (1948), 15–21. The generalization (Theorem X.47b) appeared shortly thereafter in W. Feller, "On the generation of unbounded semi-groups of bounded linear operators," *Ann. Math.* **58** (1953), 166–174, I. Miyadera: "Generation of a strongly continuous semi-group of operators," *Tôhoku Math. J.* **4** (1952), 109–114, and R. S. Phillips: "Perturbation theory for semi-groups

of linear operators," *Trans. Amer. Math. Soc.* **74** (1953), 343–369. Theorem X.47b is usually called the Hille–Yosida–Phillips theorem.

There are various other conditions besides strong continuity on $[0, \infty)$ which can be put on $T(t)$. For example, one can require:

(i) $T(t)$ is strongly measurable
(ii) $T(t)$ converges strongly to I as $t \downarrow 0$
(iiia) $\int_0^1 \|T(t)\|\, dt < \infty$
(iiib) $\lim_{\lambda\to\infty} \lambda \int_0^\infty e^{-\lambda t} T(t)\varphi = \varphi$ for all $\varphi \in X$.

It can be shown that (i) and (ii) together imply strong continuity on $[0, \infty)$. Another possible set of hypotheses is (i) and (iii). In this case $\|T(t)\|$ can be unbounded as $t \to 0$. As in the case of strong continuity, there is a theorem classifying the generators of such semi-groups. A detailed study of various continuity conditions as $t \to 0$ and the corresponding classification of generators may be found in E. Hille and R. S. Phillips: *Functional Analysis and Semi-groups*, Amer. Math. Soc. Colloquium Publication, 1957, New York.

The term "accretive" originally appeared in K. Friedrichs, "Symmetric positive linear differential equations," *Comm. Pure Appl. Math.* **11** (1958), 333–418. The study of such operators was essentially initiated by R. S. Phillips in his paper quoted above. For a semigroup e^{-tA}, Phillips calls $-A$ (rather than A) the generator. Therefore in the Hilbert space case, his generators satisfy $\mathrm{Re}(\varphi, A\varphi) \leq 0$ (rather than $\mathrm{Re}(\varphi, A\varphi) \geq 0$). He calls such operators "dissipative." The theory of dissipative operators on Banach spaces is due to G. Lumer and R. S. Phillips: "Dissipative operators in a Banach space," *Pacific J. Math.* **11** (1961), 679–698. This paper contains a counterexample which shows that a maximal accretive operator need not generate a semigroup in the Banach space case. The fact that maximal accretive operators do generate semigroups in the Hilbert space case appeared in R. S. Phillips, "Dissipative operators and hyperbolic systems of partial differential equations," *Trans. Amer. Math. Soc.* **90** (1959), 193–254.

An example of a bounded semigroup which is not a contraction semigroup is

$$\begin{pmatrix} \cos\theta & 2\sin\theta \\ -\frac{1}{2}\sin\theta & \cos\theta \end{pmatrix}$$

on $\mathbb{R}^2$. Infinite dimensional bounded semigroups which are not contractions enter in the scattering theory associated to the linearized Boltzmann equation; see Chapter XII.

In the finite-dimensional case, every semigroup obeys $\lim_{t\downarrow 0} \|T(t)\| = 1$. However, in the infinite-dimensional case this need not be true (see Example 5). When this norm condition fails there is no simple characterization of the generator directly in terms of $\ell(A\varphi)$.

Theorem X.50 is due to Gustafson: "A perturbation lemma," *Bull. Amer. Math. Soc.* **72** (1966), 334–338. The proof we give (for $a < \frac{1}{2}$) is due to E. Nelson: "Feynman integrals and the Schrödinger equation," *J. Math. Phys.* **5** (1964), 332–343, though some of the ideas already appeared in H. Trotter: "On the product of semi-groups of operators," *Proc. Amer. Math. Soc.* **10** (1959), 545–551. Nelson's and Trotter's papers also contain their proofs of the general Trotter product formula. A simplification and generalization of Trotter's theorem appears in P. R. Chernoff, "Semigroup product formulas and addition of unbounded operators," *Bull. Amer. Math. Soc.* **76** (1970), 395. The corollary to Theorem X.50 has been extended to the case where $a = 1$ in the case that X is a reflexive Banach space. This generalizes Wüst's theorem and is proven by similar methods in P. R. Chernoff, "Perturbations of dissipative operators of relative bound one," *Proc. Amer. Math. Soc.* **33** (1972), 72–74.

Theorem X.52 is due to E. Hille and R. S. Phillips (their book cited above) and K. Yosida: "On the differentiability of semi-groups of linear operators," *Proc. Japan Acad.* **34** (1958),

337–340. The proof of holomorphicity in Theorem X.55 follows E. Stein: *Topics in Harmonic Analysis*, Ann. Math. Studies, Princeton Univ. Press, Princeton, New Jersey. Dunford–Taylor type formulas for holomorphic semigroups are very important for they allow the computation of various quantities by the Cauchy integral formula.

A spectral mapping theorem for semigroups is discussed in Section XIII.8.

The connection between partial differential equations and semigroup theory goes back to J. Hadamard who noticed that the solution of the Cauchy problem has the semigroup property with respect to t: "Sur un problème mixte aux dérivées partielles," *Bull. Soc. Math. France* **31** (1903), 208–224, and "Principe de Huygens et prolongement analytique," *Bull. Soc. Math. France* **52** (1924), 241–278. But semigroup theory was not applied systematically to partial differential equations until Hille and Yosida developed the analytical tools in the late 1940's. The examples given in the text suggest that one should be able to apply semigroup theory to general second-order parabolic partial differential equations, i.e., equations of the form $\partial u(x, t)/\partial t = Au(x, t)$ where

$$A\varphi = \sum_{i,j} \frac{\partial}{\partial x_i} a_{ij}(x) \frac{\partial}{\partial x_j} \varphi(x) + \sum_i \frac{\partial}{\partial x_i} b_i(x)\varphi(x) + c(x)\varphi(x)$$

is elliptic in an appropriate sense. This is in fact true but the applications are not easy for several reasons. First, in the case of nonconstant coefficients or a bounded domain, the Fourier transform is no longer available, so one must prove that A satisfies the conditions of Theorems X.47, X.52 by a priori estimates (like Gårding's inequality) and the Hahn–Banach theorem (to show $\mathrm{Ran}(A + \lambda)$ is dense). The situation is further complicated since A (restricted to a nice domain of functions) will have many closed extensions and one must choose the "right one" as the generator. Finally, one uses a generalization of Weyl's lemma (see Section IX.6) to prove regularity. Among the fundamental papers applying semigroup techniques to parabolic equations are: W. Feller, "The parabolic differential equations and the associated semigroups of transformations," *Ann. Math.* **55** (1952), 468–519; P. Lax and A. Milgram, "Parabolic equations" in *Contributions to the Theory of Partial Differential Equations*, Princeton Univ. Press, Princeton, New Jersey, 1954; P. Lax and R. S. Phillips, "Local boundary conditions of dissipative systems of linear partial differential operators," *Comm. Pure Appl. Math.* **13** (1960), 427–455; R. S. Phillips, "On the integration of the diffusion equation with boundaries," *Trans. Amer. Math. Soc.* **98** (1961), 62–84; K. Yosida, "An abstract analyticity in time for solutions of a diffusion equation," *Proc. Japan Acad.* **35** (1959), 109–113. Certain kinds of parabolic equations which are nonlinear or where A depends on t (called evolution equations) can also be handled with semigroup methods; see A. Friedman, *Partial Differential Equations*, Holt, New York, 1969. There is an extensive literature on semigroups of nonlinear operators; see Section X.13 and its notes.

It was noticed by E. Hille in *Functional Analysis and Semi-groups*, Amer. Math. Soc. Colloquium Publication **31**, 1949, New York, that semigroup theory could also be applied to hyperbolic equations. For the wave equation with constant coefficients, the method is outlined in Problem 60. In a nonlinear context, this idea is exploited in Section X.13. For the semigroup approach to a broad class of hyperbolic problems, see R. S. Phillips, "Dissipative operators and hyperbolic systems of partial differential equations," *Trans. Amer. Math. Soc.* **90** (1959), 193–254.

The second main area of application of semigroup techniques is in probability theory. The connection between the heat equation and probability theory was discovered by A. Einstein, "Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen," *Ann. Physik* **17** (1905), 549–560. But it was not until 1952 that Feller initiated a systematic study of semigroups in probability theory in

the paper quoted above. The theory was developed in G. Hunt, "Markov processes and potentials, I," *Illinois J. Math.* **1** (1957), 44–93; II, **1** (1957), 316–369; III, **2** (1958), 151–213; and "Semigroups of measures on Lie groups," *Trans. Amer. Math. Soc.* **81** (1956), 264–293. For a description of these applications, see the probability theory books quoted in the notes to Section X.11.

We mentioned at the beginning of the section that accretive operators generalize to Banach spaces many important properties of self-adjoint operators. The main tool that does not generalize to all accretive operators is the spectral resolution. A class of "spectral operators" which do admit a kind of spectral resolution was introduced in N. Dunford: "Spectral operators," *Pacific J. Math.* **4** (1954), 321–354. An exhaustive study of such operators may be found in N. Dunford and J. Schwartz, *Linear Operators, III, Spectral Operators*, Wiley (Interscience), New York, 1971.

Section X.9 The theory of hypercontractive semigroups is an abstraction of certain developments in constructive quantum field theory. The germinal ideas appeared in E. Nelson, "A quartic interaction in two dimensions," in *Mathematical Theory of Elementary Particles*, pp. 69–73, (R. Goodman and I. Segal, eds.) M.I.T. Press, Cambridge, Massachusetts, 1966. Nelson isolated those properties of Hermite operators (Example 1) which we now call hypercontractive and used them together with the theory of Feynman path integrals to prove that certain field theoretic Hamiltonians are bounded below. This work was clarified and extended by J. Glimm, "Boson fields with nonlinear self-interaction in two dimensions," *Comm. Math. Phys.* **8** (1968), 12–25. In particular, Glimm introduced the use of the Riesz–Thorin theorem. Nelson's ideas played a role in the first proof of self-adjointness of the spatially cutoff $(\varphi^4)_2$ Hamiltonian $H_0 + H_I(g)$ by Glimm and Jaffe, "A $\lambda\varphi^4$ quantum field theory without cutoffs," *Phys. Rev.* **176** (1968), 1945–1951. Glimm and Jaffe also used graph convergence (see Section X.10) and Feynman path integrals in their proof. The basic ideas of hypercontractivity emerged from the independent work of L. Rosen and I. Segal. Rosen in "A $\lambda\varphi^{2n}$ theory without cutoffs," *Comm. Math. Phys.* **16** (1970), 157–183, gave a proof of essential self-adjointness of $P(\varphi)_2$ Hamiltonians which used hypercontractivity and Feynman path integrals. While it was not fully realized at the time, Rosen's proof depended on little more than L^p techniques and contained all the main ideas of the abstract $H_0 + V$ theory. Segal in "Notes towards the construction of nonlinear relativistic quantum fields, III: Properties of the C^*-dynamics for a certain class of interactions," *Bull. Amer. Math. Soc.* **75** (1969), 1390–1395, showed that it was possible to replace completely the use of Feynman path integrals with the Trotter product formula and that hypercontractivity could be used to provide a self-adjoint operator H which was formally $H_0 + V$. In addition, what we have called Segal's lemma appeared and it was used to simplify the earlier lower boundedness proofs of Nelson and Glimm. Segal also clarified a point in the earlier proofs concerning the question of whether the tensor product of contractions from L^2 to L^4 is necessarily a contraction. An alternative discussion of this fact can be found in the Les Houches lectures of Glimm and Jaffe quoted in the notes to Section X.7. In his fuller paper, "Construction of nonlinear quantum processes, I," *Ann. Math.* **92** (1970) 462–481, Segal supplemented this with a proof of the essential self-adjointness of $H_0 + V$ on $D(H_0) \cap D(V)$. That essential self-adjointness holds on $C^\infty(H_0) \cap D(V)$ was proven in an appendix to B. Simon, "Essential Self-Adjointness of Schrödinger Operators with Positive Potentials," *Math. Ann.* **201** (1973), 211–220. For the special case of the $(\varphi^4)_2$ Hamiltonian, this had already been proven by very different means in the Glimm and Jaffe paper mentioned above. For the case of the $(\varphi^{2n})_2$ Hamiltonian it had been proven in L. Rosen, "The $(\varphi^{2n})_2$ quantum field theory: Higher order estimates," *Comm. Pure Appl. Math.* **24** (1971), 417–457.

The theory of hypercontractive semigroups has been extended and clarified by a variety of authors. B. Simon and R. Höegh-Krohn in "Hypercontractive semi-groups and two-dimensional self-coupled Bose fields," *J. Functional Analysis* **9** (1972), 121–180, reviewed the basic theory and its use in the $P(\varphi)_2$ model, extended it in certain directions and, coined the term "hypercontractive." The special case of contractive semigroups was first emphasized for its own sake and applied in R. Höegh-Krohn, "A general class of quantum field theories without cutoff in two space-time dimensions," *Comm. Math. Phys.* **21** (1971), 244–255. Extensions to still more abstract settings can be found in I. Segal, "Construction of nonlinear local quantum processes, II," *Invent. Math.* **14** (1971), 211–241, W. Faris, "Quadratic forms and essential self-adjointness," *Helv. Phys. Acta* **45** (1972), 1074–1088 and W. Faris, "Essential self-adjointness of operators in ordered Hilbert space," *Comm. Math. Phys.* **30** (1973), 23–34. In his *Helv. Phys. Acta* paper, Faris gives an interesting "explanation" in terms of quadratic forms of why hypercontractivity should imply self-adjointness. Further applications of the hypercontractivity method in constructive quantum field theory appear in the paper of Höegh-Krohn quoted above and in A. Klein, "Self-adjointness of the locally correct generator of Lorentz transformations for $P(\varphi)_2$," in *Mathematics of Contemporary Physics* (R. Streater, ed.), Academic Press, New York, 1973, and "Quadratic expressions in a free Boson field," *Trans. Amer. Math. Soc.* **181** (1973), 439–456. Extensions of some of the ideas to fermion theories appear in L. Gross, "Existence and uniqueness of physical ground states," *J. Functional Analysis* **10** (1972), 52–109.

The simple proof of the hypercontractivity of Hermite operators which we give (Example 1) is due to E. Nelson, "The free Markov field," *J. Functional Analysis* **12** (1973), 211–227. Earlier proofs of hypercontractivity obtain Theorem X.61 in the infinite-dimensional case by a two-step process from the case of a one-dimensional one particle space. First one shows that knowing that e^{-tH_0} is bounded from L^2 to L^4 for some t and that H_0 has a gap in its spectrum above zero, one can conclude that e^{-TH_0} is actually a contraction from L^2 to L^4 for T sufficiently large. The infinite-dimensional case is then controlled by discussing tensor products of contractions from L^2 to L^4. The proof of Nelson in the one-dimensional case that we give in the text generalizes to arbitrary dimensions and so avoids the two step process. In fact, one can turn one of the steps around and prove directly that the map e^{-TH_0} is a contraction from L^2 to L^4 for suitable T. For further discussion of these points, the reader should consult Section I.5 of Simon's lectures referred to in the Notes to Section X.11.

In the above paper, Nelson also proves the following best possible bounds: Let $\mathscr{H}$ be a complex Hilbert space with distinguished complex conjugation. Let A be a bounded operator on $\mathscr{H}$ commuting with the conjugation. Let Q be the Q-space built over the Fock space on $\mathscr{H}$ according to the construction in Section 7. Then $\Gamma(A)$ is a bounded operator from $L^p(Q)$ to $L^q(Q)$ $(p \leq q)$ if and only if $\|A\| \leq \sqrt{(p-1)/(q-1)}$ and in that case it is a contraction. An alternative proof of this theorem appears in L. Gross, "Logarithmic Sobolev inequalities," *Amer. J. Math.* (to appear).

Segal's lemma can be viewed as a special case of a more general result. Let $\|\cdot\|_\infty$ denote the operator norm of $\mathscr{L}(\mathscr{H})$, then Segal's lemma says that

$$\|e^{(A+B)}\|_\infty \leq \|e^{A/2}e^{B}e^{A/2}\|_\infty$$

There is an inequality of S. Golden, "Lower bounds for the Helmholtz function," *Phys. Rev.* **137B** (1965), 1127–1128, and C. Thompson, "Inequality with applications in statistical mechanics," *J. Math. Phys.* **6** (1965), 1812–1813, which says that for A and B self-adjoint

$$\mathrm{Tr}(e^{A+B}) \leq \mathrm{Tr}(e^{A}e^{B})$$

or equivalently that

$$\|e^{A+B}\|_1 \leq \|e^{A/2}e^{B}e^{A/2}\|_1$$

It is also possible to prove that

$$\|e^{A+B}\|_p \leq \|e^{A/2}e^{B}e^{A/2}\|_p$$

for any p. The Golden–Thompson inequality is further discussed in A. Lenard, "Generalization of the Golden–Thompson inequality," *Indiana Univ. J. Math.* **21** (1971), 457–468, M. B. Ruskai, "Inequalities for Traces on von Neumann Algebras," *Comm. Math. Phys.* **26** (1972), 280–289, and C. Thompson, "Inequalities and partial orders on matrix spaces," *Indiana Univ. J. Math.* **21** (1971), 469–480.

Section X.10 The basic ideas and theorems in Section 10 are due to J. Glimm and A. Jaffe: "Singular perturbations of self-adjoint operators," *Comm. Pure Appl. Math.* **22** (1969), 401–414. Glimm and Jaffe used their results to give the first proof of the self-adjointness of the spatially cut-off $(\varphi^4)_2$ Hamiltonian (see the notes to Section X.7). The existence of the spatially cut-off Hamiltonian for the Yukawa theory was proven in two papers: Resolvent convergence was established in J. Glimm and A. Jaffe, "Self-adjointness for the Yukawa$_2$ Hamiltonian," *Ann. Physics.* **60** (1970), 321–383. That the sequence $\{H(g, n)\}_{n=1}^{\infty}$ is bounded below and densely bounded had already been proven by Glimm in "Yukawa coupling of quantum fields in two dimensions, I," *Comm. Math. Phys.* **5** (1967), 343–386. For a general discussion see the Les Houches lectures referred to in the notes to Section X.7.

The techniques used in the example can be extended to the case of the x^{2n} oscillator by using ideas from L. Rosen: "The $(\varphi^{2n})_2$ quantum field theory: Higher order estimates," *Comm. Pure Appl. Math.* **24** (1971), 417–457.

Section X.11 The first work on Wiener measure appeared in N. Wiener's paper, "Differential space," *J. Math. Phys.* **2** (1923). Wiener introduced his measure in order to make rigorous the work of Einstein and Smoluchowski on Brownian motion. The reader can find a discussion of the history of the study of Brownian motion in E. Nelson, *Dynamical Theories of Brownian Motion*, Princeton Univ. Press, Princeton, New Jersey, 1967. The construction of Wiener measure which we give is due to Nelson in "Feynman Integrals and the Schrödinger Equation," *J. Math. Phys.* **5** (1964), 332–343. The argument in Problem 64 showing that it is impossible to construct an imaginary time Feynman path (complex) measure is due to R. Cameron, "The Ilstow and Feynman Integrals," *J. Anal. Math.* **10** (1962/63), 287–361. The reader should be wary of an erroneous construction in I. Gel'fand and A. Yaglom, "Integration in function spaces and its applications to quantum physics," *J. Math. Phys.* **1** (1960), 48–69.

There is a large textbook literature on Wiener measure from a probabilistic point of view: J. Doob, *Stochastic Processes*, Wiley, New York, 1953; E. Dynkin, *Markov Processes*, Vol. I, II, Springer-Verlag, Berlin, 1965; T. Hida, *Stationary Stochastic Processes*, Princeton Univ. Press, Princeton, New Jersey, 1970; K. Itô and H. McKean, *Diffusion Processes and their Sample Paths*, Springer-Verlag, Berlin, 1965; M. Kac, *Probability and Related Topics in the Physical Sciences*, Wiley (Interscience), New York, 1959. The reader who is interested in but ignorant of the probabilistic background might profit from M. Reed, "Functional Analysis and Probability Theory," in *Constructive Quantum Field Theory* (G. Velo and A. Wightman, eds.), *Springer Lecture Notes in Physics* **25**, 1973, 1–41. A wealth of detailed information about regularity properties of Wiener measure, and in particular Theorem X.67, can be found in the Itô–McKean book.

Some of the probability literature, especially the older literature, contains technical complications which do not appear in our discussion. This is because some authors construct Wiener measure in such a way that, when translated to our terminology, it is only a Baire measure. Some nice subsets of Ω, such as Ω_α, are Borel sets but not Baire sets. The idea of avoiding some technical complications by realizing Ω as a compact product space and using regular Borel measures is due to E. Nelson, "Regular Probability Measures on Function Space," *Ann. Math.* **67** (1954), 630–643. Unfortunately, Nelson's method does not remove all measurability problems, since in further developments some non-Borel sets, such as the paths that are continuous from the right, are important.

Feynman's idea of expressing the Schrödinger dynamics in terms of a sum over histories appeared in his Princeton thesis (1942) and in R. Feynman, "Space-time approach to non-relativistic quantum mechanics," *Rev. Modern Phys.* **20** (1948), 367–387. The reader can find a detailed exposition and further developments in R. Feynman and A. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw-Hill, New York, 1965. The idea of continuing to imaginary time so that Wiener measure can be used and the Feynman–Kac formula appeared in M. Kac, "On some connections between probability theory and differential and integral equations," *Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability*, Univ. of California Press, Berkeley, 1951, 189–215. Our proof of the Feynman–Kac formula is taken from E. Nelson's *J. Math. Phys.* paper quoted above.

Path integrals have played a major role in constructive quantum field theory, especially in the recent theory of Euclidean and Markov fields. Path integral methods were first advocated in constructive quantum field theory by E. Nelson in the first paper quoted in the notes to Section X.9 and in Euclidean quantum field theory by Nelson in "Quantum fields and Markov fields," in *Partial Differential Equations* (D. Spencer, ed.) *Symp. Pure Math.* **23**, Amer. Math. Soc., Providence, Rhode Island, 1973, pp. 211–219. The reader can find further discussion of these methods and their development in *Constructive Quantum Field Theory* (G. Velo and A. Wightman eds.), *Springer Lecture Notes in Physics* **25**, 1973, and in B. Simon, *The $P(\varphi)_2$ Euclidean (Quantum) Field Theory*, Princeton Univ. Press, Princeton, New Jersey, 1974.

Section X.12 The idea of using an expansion like the Dyson expansion to find a propagator $U(t, s)$ satisfying

$$\frac{d}{dt} U(t, s) = -iH(t)U(t, s), \qquad U(s, s) = I \tag{X.163}$$

is essentially the method of successive substitution developed in the nineteenth century to solve integral equations. (X.163) is formally equivalent to the integral equation

$$U(t, s) = I - i \int_s^t H(r)U(r, s)\, dr$$

The Dyson expansion results from repeatedly substituting this expression for $U(t, s)$ under the integral. Dyson used the expansion to give a perturbation theoretic description of quantum electrodynamics in "The radiation theories of Tomonaga, Schwinger, and Feynman," *Phys. Rev.* **75** (1949), 486–502, and "The S-matrix in quantum electrodynamics," *Phys. Rev.* **75** (1949), 1736–1755.

T. Kato in "Integration of the equation of evolution in a Banach space," *J. Math. Soc. Japan* **5** (1953), 208–234, was the first to find general conditions for the solution of the evolution equation $d\varphi(t)/dt = A(t)\varphi(t)$ where $A(\cdot)$ is an unbounded-operator valued function. Since one of the main applications of this theory is in partial differential equations, there were

many special results before that. In proving Theorem X.70 we have followed closely the proof due to K. Yosida, *Functional Analysis*, 2nd ed. Springer-Verlag, Berlin, 1968, pp. 224–230. For more general results, see T. Kato, "Linear evolution equations of hyperbolic type," *J. Fac. Sci. Univ. Tokyo Sect. I, A Math.* **17** (1970), 241–258.

See B. Simon, *Quantum Mechanics for Hamiltonians defined as quadratic forms*, Princeton Univ. Press, Princeton, New Jersey, 1971, for a discussion of time-dependent form results and, in particular, extensions of Theorem X.71 to the Rollnik class.

The idea of using the Hilbert space $L^2(\mathbb{R}; \mathscr{H})$ to change time-dependent quantum Hamiltonians to time-independent ones is due to J. Howland, "Stationary scattering theory for time-dependent Hamiltonians," *Math. Ann.* **207** (1974), 315–335. One nice application of Howland's idea is to scattering theory. Let $U(t, s)$ and $U_0(t, s)$ be two unitary propagators on $\mathscr{H}$ and let $\hat{U}(\sigma)$ and $\hat{U}_0(\sigma)$ be the corresponding strongly continuous one-parameter groups on $L^2(\mathbb{R}; \mathscr{H})$. Then one can show that the wave operators for the time-dependent theory on $\mathscr{H}$ exist if and only if the usual wave operators

$$W_\pm = s - \lim_{\sigma \to \infty} \hat{U}_0(-\sigma)\hat{U}(\sigma)$$

exist on $L^2(\mathbb{R}; \mathscr{H})$. Therefore one can prove the existence of wave operators in certain theories with time-dependent Hamiltonians by reformulating as above and using the usual methods for the case where the Hamiltonians do not depend on time. For proofs of these results and those mentioned in the text, see Howland's paper.

There is another method for constructing propagators which *formally* satisfy (X.163). Namely, suppose that $\mathscr{B}$ is a Banach space whose elements are unbounded-operator valued functions on some fixed compact subinterval of $\mathbb{R}$. Suppose that $\mathscr{B}$ contains a dense subset $\mathscr{B}_0$ so that whenever $f \in \mathscr{B}_0$, (X.163) has a strict solution with $H = H_0 + f(t)$ for some fixed operator H_0. Let $U(t, s; f)$ denote the corresponding propagator. If $U(t, s; \cdot)$ is uniformly continuous on $\mathscr{B}_0$, then we can extend $U(t, s; \cdot)$ to $\mathscr{B}$ to obtain formal solutions of (X.163) for $f \in \mathscr{B}$. We will see an example of this in the appendix to Section XIII.6.

Section X.13 The original proof of the existence of global solutions of (X.138) ($m > 0$) is due to K. Jörgens, "Das Anfangswertproblem im Grossen für eine Klasse nichtlinearer Wellengleichungen," *Math. Z.* **77** (1961), 295–308. The abstract approach to such non-linear problems was developed in F. Browder, "On non-linear wave equations," *Math. Z.* **80** (1962), 249–264, and I. Segal, "Non-linear semi-groups," *Ann. Math.* **78** (1963), 339–364. A global existence theorem for the mass zero case was first proven in W. Strauss, "Decay and asymptotics for $\Box u = F(u)$," *J. Functional Analysis* **2** (1968), 409–457. The mass zero case can also be handled directly by the methods in Section X.13. The procedure is outlined in Problem 76. Similar techniques have also been applied to the coupled Maxwell–Dirac equations; see L. Gross, "The Cauchy problem for the coupled Maxwell and Dirac equations," *Comm. Pure Appl. Math.* **19** (1966), 1–15, and J. Chadam, "On the Cauchy problem for the coupled Maxwell–Dirac equations," *J. Math. Phys.* **13** (1972), 597–604; "Global solutions of the Cauchy problem for the (classical) coupled Maxwell–Dirac equations in one space dimension," *J. Functional Analysis* **13** (1973), 173–184.

The nonexistence of global solutions for certain nonlinear partial differential equations has been known for a long time; see, for example, J. Keller, "On solutions of non-linear wave equations," *Comm. Pure Appl. Math.* **10** (1957), 523–532. The example used at the end of the section was described to the authors by H. Levine. Generalizations of the example appear in his paper "Some non-existence and instability theorems for solutions of formally parabolic equations of the form $Pu_t = -Au + \tilde{F}(u)$," *Arch. Rational Mech. Anal.* **51** (1973), 371–386.

Let $\varphi(t) = \langle u(x, t), u_t(x, t)\rangle$ be the solution of the nonlinear Klein–Gordon problem described in the text and define M_t to be the mapping $M_t : \varphi(0) \to \varphi(t)$. Then M_t is a strongly continuous semigroup of bounded *nonlinear* operators. The question immediately arises whether the theory of strongly continuous semigroups of *linear* operators described in Section X.8 has a counterpart in the nonlinear case. In particular, do such nonlinear semigroups have unique infinitesimal generators? A large literature has grown about these questions. See, for example, T. Kato's article "Accretive operators and non-linear evolution equations in Banach spaces," pp. 138–161, in *Proc. Symp. Pure Math.* **18**, Part I, Amer. Math. Soc. 1970, (F. Browder, ed.) or M. Crandall's article "Semi-groups of nonlinear transformations in Banach spaces," pp. 157–171, in *Contributions to Nonlinear Functional Analysis* (E. Zarantonello, ed.), Academic Press, New York, 1971, and the references therein.

Section X.14 A fairly readable account of Hamiltonian mechanics (but with some mathematical errors) may be found in H. Goldstein, *Classical Mechanics*, Addison-Wesley, Reading, Massachusetts, 1950. A more sophisticated presentation is contained in R. Abraham, *Foundations of Mechanics*, Benjamin, New York, 1967.

The natural setting for classical mechanics is a symplectic manifold. A quadratic form q on a finite-dimensional real vector space is called **symplectic** if: (1) $q(v, w) = -q(w, v)$, (2) q is nondegenerate, i.e., $q(v, w) = 0$ for all w implies that $v = 0$. A **symplectic manifold** is a differential manifold M with a distinguished 2-form $\omega \in \Lambda^2(M)$ so that (1) $d\omega = 0$, (2) for each x, ω_x is a symplectic form on the tangent space $T_x(M)$. ω sets up a bijective map ω_*, of $T(M)$, the tangent bundle, to the cotangent bundle $T^*(M)$ by: $[\omega_*(X)][Y] = \omega(X, Y)$. Given $f, g \in C^\infty(M)$, their Poisson bracket is defined by $\{f, g\} = [\omega_*^{-1}(df)](g)$. Given a function H in $C^\infty(M)$, we define the associated Hamiltonian flow by $\dot{p}(t) = (Xp)(t)$ where X is the vector field $X = -\omega_*^{-1}(dH)$. There is a natural volume form defined by ω; namely $\wedge^n\omega \in \wedge^{2n}(M)$ if $2n = \dim(M)$. Liouville's theorem asserts that $\wedge^n\omega$ is left invariant by any Hamiltonian flow. The cotangent bundle of any manifold is a symplectic manifold in a natural way.

The L^2 version of Liouville's theorem is that L is skew symmetric. The idea of using Theorem VIII.11 to prove skew-adjointness of L can be found in W. Hunziker, "The S-matrix in classical mechanics," *Comm. Math. Phys.* **8** (1968), 282–299. The general idea of using existence theorems for first order systems to prove essential self-adjointness of differential operators is further exploited in P. Chernoff, "Essential self-adjointness of powers of generators of hyperbolic equations," *J. Functional Analysis* **12** (1973), 401–414. Chernoff uses the fact that if $U_t = e^{-iAt}$ leaves a dense set D invariant and $D \subset C^\infty(A)$, then A^n is essentially self-adjoint on D for any n. By an extra trick, this can be used to handle operators which do not appear to be squares of first order operators, e.g. $-\Delta$ on $L^2(\mathbb{R}^3)$. For let $\mathscr{H} = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3; \mathbb{R}^3) \oplus L^2(\mathbb{R}^3; \mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ and let $d(f, \mathbf{g}, \mathbf{h}, k) = (0, \operatorname{grad} f, \operatorname{curl} \mathbf{g}, \operatorname{div} \mathbf{h})$ so that $d^*d(f, \mathbf{g}, \mathbf{h}, k) = (-\Delta f, \ldots)$ and $d^2 = 0$. Let $A = d + d^*$. Then A^2 restricted to the first summand is $-\Delta$. Of course, this is a hard way to control $-\Delta$ on $L^2(\mathbb{R}^3)$ but the method allows one to prove that the Laplace–Beltrami operator is essentially self-adjoint on $C^\infty(M)$ for a wide class of Riemannian manifolds. Chernoff's methods also work to prove:

Theorem If V is in $C^\infty(\mathbb{R}^3)$ and α, β are the usual Dirac matrices, then

$$H = -\alpha \cdot i\partial + \beta m + V$$

is essentially self-adjoint on $C^\infty(\mathbb{R}^3)$.

Unlike the Schrödinger operator case, there are no growth conditions on V. As Chernoff remarks, this should not be surprising since the relativistic bound on velocities prevents finite travel time to infinity.

If H has singularities such as Coulomb singularities, one cannot ask that global solutions for (X.153) exist for all initial conditions since collisions might take place. In the multiparticle case worse horrors can be imagined. Instead, one would like to prove global solutions exist for almost all initial conditions. This is known as **almost completeness**. Almost completeness can be proven for the two-body problem using angular momentum conservation, and it can be proven for the three-body problem by using results of K. Sundman, "Le problème des trois corps," *Acta Soc. Sci. Fenn.* **35** (1909), and G. D. Birkhoff, *Dynamical Systems*, Amer. Math. Soc. Colloq. Publ. **1**, *IX* (1927). Partial results toward the N-body problem can be found in H. Pollard and D. G. Saari, "Singularities of the N-Body Problem, I, II," *Arch. Rational Mech. Anal.* **30** (1968), 263–269; in *Inequalities*, II, ed. O. Shisha, Academic Press, New York, 1970, and in D. G. Saari, "Improbability of collisions in Newtonian gravitational systems," *Trans. Amer. Math. Soc.* **162** (1971), 267–271; erratum **168** (1972), 521.

Discussions of some of the more interesting mathematical problems in classical mechanics can be found in Abraham's book and in H. Pollard, *Mathematical Introduction to Celestial Mechanics*, Prentice-Hall, Englewood Cliffs, New Jersey, 1966; C. L. Siegel and J. K. Moser, *Lectures on Celestial Mechanics*, Springer-Verlag, Berlin, 1971, and S. Sternberg, *Celestial Mechanics*, Part I, II, Benjamin, New York, 1969.

Finally we should mention the beautiful work of Lanford on existence of solutions of Newton's equations for certain systems with infinitely many particles: O. E. Lanford, III, "The classical mechanics of one-dimensional systems of infinitely many particles, I, II," *Comm. Math. Phys.* **9** (1968), 176–191; **11** (1969), 257–292.

PROBLEMS

1. (a) Let A_n be symmetric on $\mathscr{H}_n$ and D be the set of vectors in $\bigoplus_{n=1}^{\infty} \mathscr{H}_n$ of the form $\psi = (\psi_1, \psi_2, \ldots)$ where $\psi_n \in D(A_n)$ and all but finitely many ψ_n are zero. Show that $A = \sum_{n=1}^{\infty} A_n$ is symmetric on D and that $n_+(A) = \sum_{n=1}^{\infty} n_+(A_n)$, $n_-(A) = \sum_{n=1}^{\infty} n_-(A_n)$.
   (b) Show that $i\,d/dx$ on $C_0^\infty(0, \infty)$ has deficiency indices $n_+ = 0$, $n_- = 1$. Show that $i\,d/dx$ on $C_0^\infty(-\infty, 0)$ has deficiency indices $n_+ = 1$, $n_- = 0$.
   (c) Show how to construct a symmetric operator with any given pair of deficiency indices.

2. Let A be a closed symmetric operator and suppose that A has a self-adjoint extension. Is it possible for A to have a closed symmetric extension $\tilde{A}$ so that $\tilde{A}$ has no self-adjoint extensions?

3. Let $p(x)$ be a polynomial with real coefficients and let $A = p(i\,d/dx)$ with domain $C_0^\infty(0, \infty)$ in $L^2(0, \infty)$.
   (a) Prove that A is symmetric.
   (b) How are the values of $p(x)$ related to the deficiency indices of A?
   (c) Prove (without using Theorem X.3) that if $p(x)$ has only even powers then the deficiency indices of A are equal.
   (d) Prove that if the degree of p is odd, then the deficiency indices of A are unequal.

†4. Let M and N be closed subspaces of a separable Hilbert space. Prove that if $\dim M > \dim N$, then there exists a $u \in M$, $\|u\| = 1$, so that $u \in N^\perp$.

†5. Complete the analysis of Example 2 of Section X.1 by showing that the self-adjoint

extensions of A correspond to the various boundary conditions at zero stated in the example.

6. Classify the self-adjoint extensions of $-d^2/dx^2$ on $C_0^\infty(0, 2\pi)$ and interpret in terms of scattering on a circle with a distinguished point.

7. Prove that if $V(x)$ decreases as $x \downarrow 0$ in $(0, \infty)$, then $-d^2/dx^2 + V(x)$ is limit circle at zero. Hint:

   (a) First show that we may assume $V(x) < 0$ near zero without loss of generality.
   (b) Approximate $V(x)$ near zero by a decreasing step function $\tilde{V}(x)$ (infinitely many steps) so that $|V(x) - \tilde{V}(x)|$ is bounded near zero and show that $-d^2/dx^2 + V(x)$ is limit circle if and only if $-d^2/dx^2 + \tilde{V}(x)$ is limit circle near zero.
   (c) Show that $-d^2/dx^2 + \tilde{V}(x)$ is limit circle by investigating the behavior of the solutions of $\varphi''(x) = \tilde{V}(x)\varphi(x)$ and showing they are both L^2 near zero.

8. Let V be a continuous function on $(0, \infty)$ and suppose that $-d^2/dx^2 + V$ is bounded from below on $C_0^\infty(0, \infty)$.
   (a) Let E be strictly less than the lower bound of $-d^2/dx^2 + V$. Prove that no solution of $-u'' + Vu = Eu$ has more than one zero. Hint: Prove first that any $\psi \in C_0^\infty[a, b]$, $0 < a < b < \infty$, with $\psi(a) = \psi(b) = 0$ obeys

$$\int_a^b [|\psi'(x)|^2 + V(x)|\psi(x)|^2]\, dx > E \int_a^b |\psi(x)|^2\, dx$$

   (b) Now let $W \geq V$ pointwise. Prove that if $-d^2/dx^2 + V$ is limit point at 0, then so is $-d^2/dx^2 + W$.

   Remarks (1) The above is taken from the article of Kurss quoted in the notes to Section X.1. (2) There is a conjecture of K. Jörgens generalizing this: Let $M \subset \mathbb{R}^n$ be an open set whose complement has measure zero. Let V, W be continuous on M so that $-\Delta + V$ is bounded below and essentially self-adjoint on $C_0^\infty(M)$. If $W \geq V$, then $-\Delta + W$ is also essentially self-adjoint on $C_0^\infty(M)$.

9. Let $\chi(x)$ be a function on $[0, \infty)$ which is C^∞, which vanishes if $x < 1$ and which equals 1 if $x > 2$. Let $\psi \in C_0^\infty(\mathbb{R}^n)$ and let $\psi_m(x) = \psi(x)\chi(m|x|)$. If $n \geq 5$, prove that $\psi_m \xrightarrow{L^2} \psi$, $-\Delta\psi_m \xrightarrow{L^2} -\Delta\psi$, and conclude that $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n/\{0\})$ if $n \geq 5$. (See the last example in the Appendix to Section X.1.)

†10. Prove the estimate (X.17).

11. Construct a potential V on $[0, 1]$ so that $\lim_{r\to 0} V(r) = -\infty$ but with $-d^2/dx^2 + V$ in limit point case at 0 (cf. Problem 7). (Hint: Take V to be piecewise constant with steps of size $-a_n$ where $a_1 a_2^{-1}, a_3 a_2^{-1}, a_3 a_4^{-1}, \ldots, a_{2n-1}a_{2n}^{-1}, a_{2n+1}a_{2n}^{-1}$ are all very small.

†12. Fill in the details of the example of limit point–limit circle behavior for the potentials $V_{ab}(x) = 2x^{-2} - 9x^4(a - 2b\cos(2x^3))$ (see the Notes to Section X.1).

†13. Prove part (b) of Theorem X.13.

14. Let V be a measurable function on $\mathbb{R}^3$ and suppose that $V(r) \to 0$ as $r \to \infty$. If $D(V) \supset D(-\Delta)$, prove that $V \in L^2 + L^\infty$ and thus $< < -\Delta$. (Thus the "potentials" for which one can use Rellich's theorem are precisely the class $L^2 + L^\infty$.)

15. Show that $A = -d^2/dx^2 + V$ is form-bounded from below on $C_0^\infty(0, \infty)$ if $V(x) \geq -1/4x^2$ and is not form-bounded from below if $V(x) \leq c/x^2$ with $c < -\frac{1}{4}$.

16. Let $E > 0$. Prove directly using the kernel for $(-\Delta + E)^{-1}$ that $V(-\Delta + E)^{-1}$ is bounded if $V \in L^2(\mathbb{R}^3)$ and that $\|V(-\Delta + E)^{-1}\| \to 0$ as $E \to \infty$. Conclude from this (without the Sobolev estimate) that $V << -\Delta$.

17. Let V be in the Rollnik class. Prove that:
(a) $\| |V|^{1/2}(-\Delta + E)^{-1}|V|^{1/2} \| \to 0$ as $E \to \infty$
(b) $\| |V|^{1/2}(-\Delta + E)^{-1/2} \| \to 0$ as $E \to \infty$
(c) $\|(-\Delta + E)^{-1/2}|V|(-\Delta + E)^{-1/2}\| \to 0$ as $E \to \infty$
(d) $V \in R$ implies that $V << -\Delta$.

18. Let A and C be essentially self-adjoint on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. Suppose that $B << A$ and that D is C-bounded. Prove that $A \otimes C + B \otimes D$ is essentially self-adjoint on $D(A) \otimes D(C)$.

19. Let A be self-adjoint and let B be symmetric. Suppose that B is A-bounded with relative bound equal to a. Prove that

$$a = \lim_{n \to \infty} \|B(A + in)^{-1}\|$$

20. Let A be self-adjoint. An operator B with $D(B) \supset D(A)$ is called **A-compact** if $B(A - z)^{-1}$ is compact for all $z \in \rho(A)$.
(a) Prove that B is A-compact if $B(A - z)^{-1}$ is compact for one $z \in \rho(A)$.
(b) Suppose that B is symmetric and A-compact. Prove that $B << A$. (Hint: use Problem 19.)

21. Let $\mathscr{H}_m$, $m = \{0, \pm 1, \ldots\}$ be the scale of spaces associated to a positive operator A.
(a) Prove that B is A-compact if and only if B is a compact operator from $\mathscr{H}_{+2}$ to $\mathscr{H}$.
(b) Let β be a symmetric quadratic form which is form bounded with respect to A. Prove that if β defines a compact operator from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$, then $\beta << A$.
*(c) Let B be a self-adjoint operator which is A-compact. Prove that B defines a compact operator from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$.

22. Use Konrady's trick to prove that $-d^2/dx^2 + p(x)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$, where $p(x) = ax^6 + \sum_{i=0}^5 c_i x^i$ and $a > 0$ is sufficiently small.

23. (a) Prove that for any $a > 1$, there is some b, so that for all $\psi \in \mathscr{S}(\mathbb{R})$

$$\|(p^2 + x^2)\psi\|^2 + \|x^4\psi\|^2 \leq a\|(p^2 + x^2 + x^4)\psi\|^2 + b\|\psi\|^2$$

where $p = -i\, d/dx$.
(b) Knowing that $p^2 + x^2 + x^4$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$, conclude that it is self-adjoint (in particular, it is closed) on $D(p^2 + x^2) \cap D(x^4)$.
(c) In a similar way prove $D(p^2 + x^2) = D(p^2) \cap D(x^2)$ and conclude that

$$D(p^2 + x^2 + x^4) = D(p^2) \cap D(x^4)$$

24. The purpose of this problem is to prove (without using Theorem X.28) that if $V(x)$ is C^∞, real-valued, and bounded below on $\mathbb{R}^n$, then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.
(a) Observe that we may assume $V(x) \geq 1$ and prove

$$D((-\Delta + V)^*) = \{\psi \,|\, \psi \in L^2, -\Delta\psi + V\psi \in L^2\}$$

where $-\Delta + V$ acts in the sense of distributions.

(b) Explain why every weak solution of $-\Delta\psi + V\psi = 0$ is a C^∞ function.
(c) Show that every weak solution of $\Delta\psi = V\psi$ satisfies

$$\Delta|\psi(x)|^2 \geq |\psi(x)|^2$$

(d) If $\psi \in \mathrm{Ker}((-\Delta + V)^*)$, define $F(r) = \int_{|x|^2=r} |\psi(x)|^2\, d\Omega$ where $d\Omega$ is the usual measure on the sphere. Show by an integration by parts that F is monotone increasing.
(e) Conclude that $\psi = 0$, so $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

25. (Stieltjes moment condition)
(a) Prove that a sequence of real numbers $\{a_n\}_{n=0}^\infty$ are the moments of a measure with support on the positive half line if and only if

$$\sum_{n,m=0}^{N} \bar{\beta}_n \beta_m a_{n+m} \geq 0 \qquad \text{and} \qquad \sum_{n,m=0}^{N} \bar{\beta}_n \beta_m a_{n+m+1} \geq 0$$

for all N and all $\langle \beta_1, \ldots, \beta_N \rangle \in \mathbb{C}^N$. (Hint: Mimic the proof of the Hamburger moment condition (Section X.1) but use the Friedrichs extension.)
(b) Prove that if in addition to the positivity requirements the a_n satisfy $|a_n| \leq CD^n(2n)!$, then the solution of part (a) is unique. (Hint: Use Theorem X.40.)

26. Construct a semibounded symmetric operator which has a nonsemibounded self-adjoint extension.

27. Let A be a symmetric operator with an invariant domain.
(a) Let B be the Friedrichs extension of $A^2 \upharpoonright D(A)$. Prove that $B = A^*\bar{A}$.
(b) Let $C = \bar{A}A^*$. Prove that C is a self-adjoint extension of $A^2 \upharpoonright D(A)$ and that one has $Q(C) = D(A^*)$.

28. Let A be a symmetric operator and suppose that $D(A^2)$ is dense. Prove that if A^2 is essentially self-adjoint on $D(A^2)$, then A is essentially self-adjoint. (Hint: First prove $(A^*)^2 \subset (A^2)^*$.)

29. Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Prove that $\psi \in \mathscr{H}$ is an analytic vector for A if and only if the function $f(t) = e^{itA}\psi$ is the restriction to the real axis of a function analytic in the strip $|\mathrm{Im}\, t| < b$ for some $b > 0$.

30. The purpose of this problem is to prove von Neumann's theorem (Theorem VIII.14). Let U, V obey the Weyl relations $U(t)V(s) = e^{its}V(s)U(t)$. Let $\alpha > 0$ and let f be of the form $f(s, t) = s^n t^m \exp(-\alpha(s^2 + t^2))$. For $\psi \in \mathscr{H}$, define:

$$W_\psi(f) = \int f(s, t)U(t)V(s)\psi\, ds\, dt$$

(a) Prove that $\{W_\psi(f) | \psi \in \mathscr{H}\}$ is total in $\mathscr{H}$. Let D be the finite linear span of $\{W_\psi(f)\}$.
(b) Prove that $U(t_0)W_\psi(f) = W_\psi(f(s, t - t_0))$ and that

$$V(s_0)W_\psi(f) = W_\psi(f(s - s_0, t)e^{-its_0})$$

and use this to prove that each W_ψ is an analytic vector for P and for Q.
(c) Prove that $PW_\psi(f) = W_\psi(i\,\partial_t f)$ and that $QW_\psi(f) = W_\psi(i\,\partial_s f) + W_\psi(-tf)$. Use this to prove that D is a set of analytic vectors for $N = \frac{1}{2}(P^2 + Q^2 - 1)$.
(d) Let $A = \frac{1}{2}\sqrt{2}\,(Q + iP)$. Prove that A and A^* are defined on $C^\infty(N)$ and map $C^\infty(N)$ into itself. (Hint: Use the method of Section X.5.) Prove that $N = A^*A$ on vectors in $C^\infty(N)$.

(e) Let $\psi \neq 0$ be in the range of a spectral projection $E_{[n-1,n]}$ for N. Prove that $N^m A\psi = A(N-1)^m\psi$.

(f) Under the conditions in (e), prove that

$$(n-1)(n-2)^m\|\psi\|^2 < (A\psi, N^m A\psi) \leq n(n-1)^m\|\psi\|^2$$

and conclude that $A\psi$ is in the range of the spectral projection $E_{[n-2,n-1]}$ and that $A\psi \neq 0$ if $n \geq 1$.

(g) If ψ obeys the conditions of (e), prove that $A^n\psi = \varphi \neq 0$ but $A\varphi = 0$. Prove that $N\psi = n\psi$ and that $\psi = (1/n!)(A^*)^n\varphi$.

(h) By picking an orthonormal basis for $\{\varphi | A\varphi = 0\}$, complete the proof of von Neumann's theorem.

31. Use the ideas of Problem 30 to prove that the Hermite functions are a basis for $L^2(\mathbb{R}, dx)$.

†*32.* Work out the details of all the statements about lower bounds and deficiency indices in Example 1 of Section X.3.

33. (a) Let $A_1, \ldots, A_n$ be an n-tuple of symmetric operators on a dense set $D \subset \mathscr{H}$. Call $\langle A_1, \ldots, A_n\rangle$ closed if D with the norm $|||\psi||| = \sum_{i=1}^n \|A_i\psi\| + \|\psi\|$ is a Banach space. Prove that any such n-tuple has a smallest closed extension.

(b) Let $\langle A_1, \ldots, A_n\rangle$ be an n-tuple of symmetric operators closed in the sense of (a). Prove that $\sum_{i=1}^n A_i^* A_i$ defined on $\{\psi | \psi \in D; A_i\psi \in D(A_i^*)\}$ is self-adjoint.

(c) Let $\mathbf{A}(x)$ be an $\mathbb{R}^3$-vector-valued function on $\mathbb{R}^3$ which is locally square integrable and let $V(x)$ be a positive function which is locally L^1. Find a "natural" definition of

$$H = -\frac{1}{2m}\left(\frac{1}{i}\nabla - \frac{e}{c}\mathbf{A}\right)^2 + V$$

†*34.* Let q_n be a counting of the rationals and let a be a quadratic form on $C_0^\infty(\mathbb{R})$ given by

$$a(\psi, \varphi) = \sum_{n=0}^{\infty} 2^{-n}\overline{\psi(q_n)}\varphi(q_n)$$

Let $N = -d^2/dx^2 + 1$ on $L^2(\mathbb{R})$.

(a) Prove that for all $\varphi, \psi \in C_0^\infty(\mathbb{R})$, and some constant D

$$|a(\varphi, \psi)| \leq D\|N^{1/2}\varphi\|\,\|N^{1/2}\psi\|$$

and conclude that there is an operator A on $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ associated to a.

(b) Prove that $\hat{A}$ has $D(\hat{A}) = \{0\}$.

35. Let N be an operator which is self-adjoint with $N \geq 1$. Suppose that a is a symmetric quadratic form with form domain $Q(a) = D(N^2)$ with (i) $\pm a \leq cN^2$; (ii) $\pm i[N, a] \leq dN$ (as forms on $D(N^2)$ where we use (i) to extend a to a form on $D(N)$).

(a) For $\varphi, \psi \in D(N^2)$, prove that

$$a(\varphi, \psi) = a(N^{-1}\varphi, N\psi) - [a, N](N^{-1}\varphi, \psi)$$

and conclude that $|a(\varphi, \psi)| \leq (c+d)\|\varphi\|\,\|N^2\psi\|$.

(b) Prove that there is a symmetric operator A defined on $D(N^2)$ so that AN^{-2} is bounded and $(\varphi, A\psi) = a(\varphi, \psi)$ for all $\varphi, \psi \in D(N^2)$.

(c) For each $\lambda > 0$, define a quadratic form $\delta(\lambda)$ on $\mathscr{H}$ by

$$\delta(\lambda) = \lambda^2(N+\lambda)^{-2}[N, a](N+\lambda)^{-1} + \lambda^2(N+\lambda)^{-1}[N, a](N+\lambda)^{-2}$$

Prove that $\delta(\lambda)$ is an antisymmetric form which is bounded with $\|\delta(\lambda)\| \leq 2d$. Let $\Delta(\lambda)$ denote the skew-symmetric operator associated to δ.

(d) Prove that $\|\Delta(\lambda)N^{-1}\| \to 0$ as $\lambda \to \infty$ and conclude that $\Delta(\lambda) \to 0$ strongly as $\lambda \to \infty$.

(e) By taking matrix elements, prove that for any $\theta \in D(A^*)$,

$$A[\lambda^2(N+\lambda)^{-2}]\theta = [\lambda^2(N+\lambda)^{-2}]A^*\theta + \Delta(\lambda)\theta$$

(f) Let $\theta(\lambda) = \lambda^2(N+\lambda)^{-2}\theta$. Prove that $\theta(\lambda) \to \theta$, $A\theta(\lambda) \to A^*\theta$ and conclude that A is essentially self-adjoint.

Remark The above generalization of the Nelson commutator theorem is a special case of a theorem of Jaffe which allows $\pm a \leq cN^2$ to be replaced by $\pm a \leq cN^m$ for some fixed m; see the paper of McBryan quoted in the Notes to Section X.5.

36. Suppose that each component of $\mathbf{A}$ is a real-valued function in $L^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and that V is in $R + L^\infty(\mathbb{R}^3)$ where R is the Rollnik class. For $\varphi, \psi \in Q(\Delta)$, define

$$M(\varphi, \psi) = \left(\frac{1}{i}\nabla\varphi, \mathbf{A}\psi\right) + \left(\mathbf{A}\varphi, \frac{1}{i}\nabla\psi\right) + (\mathbf{A}\varphi, \mathbf{A}\psi)$$

Prove that M is a $-\Delta$ form bounded perturbation with relative bound zero and conclude that there is a unique self-adjoint operator H with $Q(H) = Q(\Delta)$ and

$$(\varphi, H\psi) = (\varphi, -\Delta\psi) + M(\varphi, \psi) + (\varphi, V\psi)$$

37. Extend Theorem X.22 and Problem 36 to the many-body case.

38. Use the methods of Sections X.4 and X.5 to prove that the $L^2(\mathbb{R}^{3N+3})$ operator

$$-(2M_0)^{-1}(\partial_0 - ie\mathbf{A})^2 - (2m)^{-1}\sum_{n=1}^{N}(\partial_n - ie\mathbf{A})^2 - Ne^2\sum_{n=1}^{N}|\mathbf{x}_i - \mathbf{x}_0|^{-1}$$

$$+\frac{1}{2}e^2\sum_{n\neq m}|\mathbf{x}_n - \mathbf{x}_m|^{-1} + e\mathbf{E}_0 \cdot \left(\mathbf{x}_0 - \sum_{n=1}^{N}\mathbf{x}_n\right)$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3N+3})$ if $\mathbf{A} \in C^1(\mathbb{R}^3)_{\text{loc}}$.

†*39.* Show by example that a self-adjoint operator A may have a domain of essential self-adjointness which is disjoint from $D(A^2)$.

40. Let $A = i\,d/dx$ with domain $D(A) = \{\varphi \in L^2[0, 1] \mid \varphi \in AC[0, 1],\ \varphi' \in L^2[0, 1],$ and $\varphi(0) = \varphi(1)\}$. A is self-adjoint. Let $D = \{\varphi \in L^2[0, 1] \mid \varphi$ has an analytic periodic extension to all of $\mathbb{C}$ with x-period one and $\varphi(0) = 0 = \varphi(1)\}$.

(a) Prove that D is a dense set of analytic vectors for A.

(b) Is $A \restriction D$ essentially self-adjoint?

41. Let $U(a, R)$ be a one-dimensional representation of the three-dimensional special Euclidean group. By showing that the spectrum of the momentum must be rotation invariant and using the fact that $SO(3)$ has no nontrivial one-dimensional representations, prove that $U(a, R) = 1$ for all a, R.

†*42.* The purpose of this problem is to prove Theorem X.40.

(a) Let φ be a semianalytic vector for $A \geq 0$. Suppose that $\tilde{A} \geq 0$ is a self-adjoint extension of A_φ on $\mathscr{H}_\varphi$ (for notation see Section X.6). Prove that $\cos(t\tilde{A}^{1/2})$ is

uniquely determined by the numbers $(\psi, A_\varphi^n \psi)$, where $\psi \in D_\varphi$. Conclude that there is at most one positive self-adjoint extension of A_φ.

(b) Prove that there is at most one semibounded extension of A_φ.

(c) Use Theorem X.24 to conclude that A_φ is essentially self-adjoint.

(d) Prove Theorem X.40 by using Nussbaum's lemma.

†43. (a) Prove part (b) of Theorem X.41. (Hint: let $\mathscr{P}_n$ be the polynomials of degree n in $\Phi_S(f)$. Prove by induction that $\mathscr{P}_n\Omega_0$ is dense in $\mathscr{H}_s^{(n)}$).

(b) Prove part (a) (iii) of Theorem X.43.

‡44. Prove that the map $E: \mathscr{S}_{\mathbb{R}}(\mathbb{R}^4) \to L^2(H_m, d\Omega_m)$ defined by $Ef = \sqrt{2\pi}\, \hat{f} \restriction H_m$ has a dense range.

45. Prove that as quadratic forms on $D_{\mathscr{S}} \times D_{\mathscr{S}}$,

$$N = \int_{\mathbb{R}^3} a^\dagger(p)a(p)\, dp$$

$$H_0 \equiv d\Gamma(\mu) = \int_{\mathbb{R}^3} \mu(p)a^\dagger(p)a(p)\, dp$$

†46. Prove (X.76), (X.78), (X.79).

47. Prove that if $g \in L^p(\mathbb{R})$, $1 < p \leq 2$, then $\hat{g}(\sum k_i) \prod_{i=1}^n \mu(k_i)^{-1/2} \in L^2(\mathbb{R}^n)$. (Hint: Use the Hausdorff-Young and Young inequalities.)

48. Let $\mathscr{H}$ be a Hilbert space and $A_1, A_2, \ldots$ a sequence of commuting self-adjoint operators. Suppose that D is a dense domain contained in the domain of each A_i which is invariant under each A_i. Let $\psi_0 \in D$ and define $\circ A_1 \cdots A_n \circ$ recursively by setting $\circ A_1 \cdots A_n \circ = A_1 \cdots A_n + P(A_1, \ldots, A_n)$ where $P(A_1, \ldots, A_n)$ is a polynomial of total degree $n-1$ and individual degree 1, so that

$$((\circ A_1 \cdots A_n \circ)\psi_0, (\circ A_{i_1} \cdots A_{i_m} \circ)\psi_0) = 0$$

for each $\{i_1, \ldots, i_m\} \subsetneq \{1, \ldots, n\}$ and $((\circ A_1 \cdots A_n \circ)\psi_0, \psi_0) = 0$.

(a) Show that $\circ A_1 \cdots A_n \circ$ is uniquely defined for each $n \geq 1$.

(b) If φ is the canonical field on $\mathscr{F}_s(\mathscr{H})$ and $f_n \in \mathscr{H}_C$, and $\psi_0 = \Omega_0$, show that

$$\circ \varphi(f_1) \cdots \varphi(f_n) \circ = :\varphi(f_1) \cdots \varphi(f_n):$$

(c) Show that for each n, the Wick power of the canonical field is the regular power plus a polynomial of lower degree in the regular powers and vice versa.

(d) Show that $:\varphi_m(x, n)^4:$ (introduced in the proof of Theorem X.45) may be written

$$:\varphi_m(x, n)^4: = \varphi_m(x, n)^4 - c_1\varphi_m(x, n)^2 - c_2$$

where c_1 and c_2 depend on n but not on x.

49. Let A be the infinitesimal generator of a contraction semigroup on a Banach space X. Show that for all $\varphi \in X$, $\lim_{n\to\infty} (1 + (t/n)A)^{-n}\varphi = e^{-tA}\varphi$. *Reference*: Kato's book on perturbation theory, pp. 478–480.

50. Let A be an accretive operator on a Hilbert space $\mathscr{H}$.

(a) Show that $J = (I - A)(I + A)^{-1}$ is a (not necessarily everywhere defined) closed contraction operator.

(b) Show that the accretive extensions of A are in one-to-one correspondence with the contraction extensions of J.
(c) Use parts (a) and (b) to prove that a maximal accretive operator on a Hilbert space generates a contraction semigroup.

51. Let $T(t)$ be a strongly continuous semigroup on a Banach space X. Define $\omega_0 = \inf_{t>0} t^{-1} \log\|T(t)\|$.
(a) Prove that $\omega_0 = \lim_{t\to\infty} t^{-1} \log\|T(t)\|$.
(b) Show that for any $\omega_1 > \omega_0$, there is a constant M so that $\|T(t)\| \le Me^{\omega_1 t}$ for all $t > 0$.

52. Let A be an accretive operator on a Banach space X. Prove that A is closable. (Hint: If A is not closable, there exists a sequence $\varphi_n \in D(A)$ such that $\varphi_n \to 0$ and $A\varphi_n \to \psi$ with $\|\psi\| = 1$. Let $\eta \in D(A)$ with $\|\eta\| = 1$ and $\|\eta - \psi\| > \frac{1}{2}$. Let ℓ_n be a sequence of normalized tangent functionals to the vectors $\eta + c\varphi_n$. Use Alaoglu's theorem to derive a contradiction for appropriate $c > 0$.)

53. Prove that $e^{\Delta t}$ is a continuous L^p-contractive semigroup by using Young's inequality and the explicit form for the kernel.

54. Let $q(x)$ be a bounded, real-valued, continuous function. Prove that $e^{t(\Delta - q)}$ is positivity preserving on $C_\infty(\mathbb{R}^n)$.

55. Fill in the details in the proof of Theorem X.47b.

†56. Prove Theorem X.53 by using the technique of Theorems X.12 and X.50. (Hint: First show that given $\theta_1 < \theta$, one can choose $\omega > 0$ so that $\|B(A - (\lambda - \omega))^{-1}\| \le \frac{1}{2}$ for all $\lambda \notin \overline{S}_{\pi/2-\theta_1}$.)

57. (a) Prove directly that

$$(e^{z\Delta}f)(x) = (4\pi z)^{-n/2} \int_{\mathbb{R}^n} \exp\left(-\frac{|x-y|^2}{4z}\right) f(y)\, dy$$

is a bounded holomorphic semigroup of angle $\pi/2$ on $C_\infty(\mathbb{R}^n)$.
(b) Prove directly that as an operator on $C_\infty(\mathbb{R}^n)$,

$$\|\partial_i e^{t\Delta}\| \le Ct^{-1/2}$$

Conclude that $\partial_i(-\Delta + 1)^{-1}$ is bounded on $C_\infty(\mathbb{R}^n)$ so that $D(\Delta) \subset D(\partial_i)$ as operators on $C_\infty(\mathbb{R}^n)$.

†58. Prove Corollary 2 to Theorem X.52.

59. Let $S(s) = e^{-sB}$ and $T(t) = e^{-tA}$ be contraction semigroups on a Banach space X. Suppose that for all $s > 0$ and $t > 0$, $e^{-sB}e^{-tA} = e^{-tA}e^{-sB}$. Then $R(t) = e^{-tB}e^{-tA}$ is a strongly continuous semigroup. Prove that the generator C of $R(t)$ satisfies

$$(I + C)^{-1} = \int_{-\infty}^{\infty} (\tfrac{1}{2} + iy + A)^{-1}(\tfrac{1}{2} - iy + B)^{-1}\, dy$$

60. Let $K_1(\mathbb{R}^3)$ be the closure of $\mathscr{S}(\mathbb{R}^3)$ in the norm $\|\varphi\|_1^2 = \int_{\mathbb{R}^3} |\nabla\varphi|^2\, dx$ and let $\mathscr{H} = K_1(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ with inner product

$$(\langle f_1, f_2\rangle, \langle g_1, g_2\rangle) = \int_{\mathbb{R}^3} (\overline{\nabla f_1} \cdot \nabla g_1 + \overline{f_2}\, g_2)\, dx$$

Let A be the operator $\begin{pmatrix} 0 & I \\ \Delta & 0 \end{pmatrix}$ with domain consisting of all pairs $\langle f_1, f_2 \rangle$ with $f_1, f_2 \in \mathscr{S}(\mathbb{R}^3)$.

(a) Show that iA is symmetric.

(b) Show that iA is essentially self-adjoint by showing that its deficiency indices are $\langle 0, 0 \rangle$.

(c) Show that $D(\overline{(iA)}) = \{\langle f_1, f_2 \rangle \mid \Delta f_1 \in L^2(\mathbb{R}^3), f_2 \in K_1(\mathbb{R}^3)\}$.

(d) Let $U(t) = e^{i(\overline{iA})t} = e^{-\overline{tA}}$ and for $\langle f_1, f_2 \rangle \in D(\overline{A})$ set $\langle u_1(x, t), u_2(x, t) \rangle = U(t)\langle f_1, f_2 \rangle$. Prove that

$$\left(\frac{\partial^2}{\partial t^2} - \Delta\right) u_1(x, t) = 0, \qquad \|u_1(x, t) - f_1(x)\|_{L^2(\mathbb{R}^3)} \to 0$$

and

$$\left\| \frac{\partial}{\partial t} u_1(x, t) - f_2(x) \right\|_{L^2(\mathbb{R}^3)} \to 0 \qquad \text{as} \quad t \to 0$$

61. Let $\{T(t)\}_{t \geq 0}$ be a family of operators on a reflexive Banach space X so that

(i) $T(t + s) = T(t)T(s)$

(ii) $\bigcup_{t>0} \text{Ran}(T(t))$ is dense in X

(iii) $\ell(T(t)\varphi)$ is measurable for each fixed $\varphi \in X$ and $\ell \in X^*$

(iv) $\|T(t)\| \leq 1$ for all t.

Prove that $T(t)$ is strongly continuous. (Hint: Mimic the proof of Theorem VIII.9.)

†*62.* Let $A^\dagger$ and A be the operators defined in Example 2 of Section 6 and let $H_0 = A^\dagger A + \frac{1}{2}$, $V = x^4 = ((A + A^\dagger)/\sqrt{2})^4$.

(a) Prove that

$$\|[H_0^{3/2}, [H_0^{3/2}, V]]\varphi\| \leq e_1 \|H_0^3 \varphi\| + e_2 \|\varphi\|$$

for some constants e_1 and e_2. (Hint: Look at each term in V separately and for each term prove the estimate on the nth Hermite function.)

(b) Use (a) to show that for each $\varepsilon > 0$ there is an M_2 so that (X.109) holds.

(c) Use similar methods to prove (X.110).

63. (a) Prove that the weak topology on the unit ball in a separable Hilbert space is metrizable.

(b) Conclude that the balls in a separable Hilbert space are weakly sequentially complete.

64. Let

$$\tilde{p}(x, y; t) = (4\pi D t)^{-n/2} e^{-|x-y|^2/4Dt}$$

for some D with $\text{Re } D \geq 0$, $D \neq 0$. Suppose that there is a *signed* measure μ on the path space Ω of Section X.11 so that $\int \varphi \, d\mu$ is given by the right-hand side of (X.122) but with p replaced by $\tilde{p}$ for $\varphi \in C_{\text{fin}}(\Omega)$. Given $t_1, \ldots, t_n$, let $C^{t_1, \ldots, t_n}$ denote those functions in $C_{\text{fin}}(\Omega)$ of the form $F(\omega(t_1), \ldots, \omega(t_n))$.

(i) If $\text{Re } D = 0$, prove that

$$\sup\left\{\left|\int \varphi \, d\mu\right| \,\middle|\, \|\varphi\|_\infty = 1, \varphi \in C^{t_1}(\Omega)\right\} = \infty$$

and conclude that no such signed measure exists.

(ii) If $\operatorname{Re} D > 0$, prove that

$$\sup\left\{\left|\int \varphi \, d\mu\right| \,\middle|\, \|\varphi\|_\infty = 1, \varphi \in C^{t_1,\cdots,t_n}(\Omega)\right\} = (|D|/\operatorname{Re} D)^n$$

and conclude that no such signed measure exists unless $\operatorname{Im} D = 0$.

65. Let Ω_α denote the Hölder continuous paths of order α for some $\alpha < \frac{1}{2}$. Define functions x and x_n from $\Omega \times [0, \infty)$ to $\mathbb{R}$ by

$$x(\omega, t) = \begin{cases} \omega(t) & \text{if } \omega \in \Omega_\alpha \\ 0 & \text{otherwise} \end{cases}$$

and let

$$x_n(\omega, t) = \begin{cases} \omega(m/n) & \text{if } \omega \in \Omega_\alpha \text{ and } m/n \le t < (m+1)/n \\ 0 & \text{otherwise} \end{cases}$$

(a) Prove that each $x_n(\omega, t)$ is Borel measurable.
(b) Prove that $x_n(\omega, t) \to x(\omega, t)$ pointwise on $\Omega \times [0, \infty)$ as $n \to \infty$ and conclude that $x(\cdot, \cdot)$ is Borel measurable.
(c) Let S have Lebesgue measure zero in $\mathbb{R}^3$. Let $\Omega_S = \{\langle \omega, t\rangle \in \Omega_\alpha \times [0, \infty) | \omega(t) \in S\}$. Prove that Ω_S is measurable.
(d) For each $t > 0$, prove that $\mu_x\{\omega \mid \langle \omega, t\rangle \in \Omega_S\} = 0$ and conclude by Fubini's theorem that $(d\mu_x \otimes dt)(\Omega_S) = 0$.
(e) Complete the proof of the lemma following Theorem X.67 by showing that for almost all $\omega \in \Omega$, $\{t \mid \langle \omega, t\rangle \in \Omega_S\}$ has Lebesgue measure zero.

66. Let H_0 be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Let $t \to V(t)$ be a strongly continuous map from $\mathbb{R}$ into the bounded operators on $\mathscr{H}$ satisfying:

(1) For each t, $V(t)$: $D(H_0) \to D(H_0)$ and $[H_0, V(t)]$ is a bounded operator.
(2) $\|[H_0, V(t)]\|$ is locally bounded.

(a) Using the Dyson expansion and the interaction representation prove that if $\psi \in H_0$, then $\varphi_s(t) = e^{-iH_0 t}\tilde{U}(t, s)\psi$ is a strong solution of

$$\frac{d}{dt}\varphi_s(t) = -i(H_0 + V(t))\varphi_s(t), \qquad \varphi_s(s) = \psi$$

(b) Prove the conclusion of (a) by showing that $H_0 + V(t)$ satisfies the hypotheses of Theorem X.70.

67. Let H_0 be the self-adjoint extension of $-d^2/dx^2$ on $L^2[0, \pi]$ corresponding to the boundary conditions $\varphi(0) = 0 = \varphi(\pi)$. Let $V(x, t) = \alpha(t)x$ where $\alpha(t)$ is a positive C^∞ function with support in the interval $[0, t_0]$ satisfying $\int \alpha(t)\, dt = 1$.
(a) Using the method of Example 1 in Section X.12, find upper and lower bounds for the transition probability at t_0 from the first excited state to the ground state.
(b) Why are these estimates valid for all $t > t_0$ also?

†68. (a) Prove that the hypotheses on $q(x, t)$ in Example 2 of Section 12 permit the application of Theorem X.70.
(b) Prove that the hypotheses on $t \to V_1(t)$ and $t \to V_2(t)$ in Theorem X.71 permit the application of Theorem X.70.

69. Let $U(t, s)$ be a strongly continuous unitary propagator on a Hilbert space $\mathscr{H}$. Prove that

$$(\tilde{U}(\sigma)f)(t) = U(t, t-\sigma)f(t-\sigma)$$

is a strongly continuous unitary group on $L^2(\mathbb{R}; \mathscr{H})$.

70. Under suitable hypotheses on $V(x, t)$, prove a Feynman-Kac formula in the time-dependent case.

71. Show that if f and g are real-valued, then the components of $W(t)\langle f, g\rangle$ are real-valued for each t where $W(t)$ is the unitary group defined in Section X.13. Use this to show that the solution of (X.138) is real-valued if the initial data are real-valued.

*72. Suppose that the hypotheses of Theorem X.72 hold. Extend J to a map $\tilde{J}$ from $\mathscr{H}$ to $\mathscr{H}$ obeying (H_0) and $(H_0^{\frac{1}{2}})$. Suppose that $\varphi(s)$ is a continuous $\mathscr{H}$-valued function on $[0, t]$ obeying the integral equation (X.143) (with $\tilde{J}$ replacing J). Prove that φ is actually $D(A)$-valued and continuously differentiable and satisfies (X.142) if $\varphi(0) \in D(A)$.

73. Prove all the higher order estimates needed in the proof of Theorem X.76.

74. Show that if every local solution $\varphi(t)$ of (X.142) obeys $\operatorname{Re} \int_0^t (J(\varphi(s)), \varphi(s))\, ds \leq 0$, then the solutions exist globally in t.

75. By using the theorems in Section X.12 prove global existence, uniqueness, smoothness, continuous dependence on the initial data, and finite propagation speed for the equation

$$u_{tt} - \Delta u + m^2 u = -\lambda u^{2n+1}$$
$$u(0, x) = f(x)$$
$$u_t(0, x) = g(x)$$

where $\lambda > 0$, $x \in \mathbb{R}^2$, and $n = 0, 1, 2, \ldots$.

76. In order to handle the mass zero equation in $\mathbb{R}^3$,

$$u_{tt} - \Delta u = -\lambda |u|^2 u, \qquad \lambda > 0$$
$$u(0, x) = f(x)$$
$$u_t(0, x) = g(x)$$

we rewrite it with a linear term added to both sides,

$$u_{tt} - \Delta u + m^2 u = -\lambda |u|^2 u + m^2 u, \qquad m > 0$$

and then formulate the problem as a first-order equation in t as in Section X.13:

$$\varphi'(t) + iA\varphi(t) = J(\varphi(t))$$
$$\varphi(0) = \langle f, g\rangle$$

where $J(\varphi(t)) = J(\langle u(t), v(t)\rangle) = \langle 0, -\lambda |u|^2 u + m^2 u\rangle$.

(a) Show that the estimates of Lemmas 4 and 5 hold for this new J so by Theorem X.72 we get local existence and uniqueness.

(b) Prove that on any interval $[0, T)$ where a solution exists the energy

$$E(t) = \frac{1}{2}\int_{\mathbb{R}^3} (|\nabla u|^2 + |u_t|^2)\, dx + \frac{\lambda}{4}\int |u|^4\, dx$$

is constant.

(c) Prove that on any interval $[0, T)$ where a solution exists, $\|u(t)\|_2 \leq C + t\sqrt{2E}$.
(d) Use parts (b) and (c) to show that if $T < \infty$, then the solution $\varphi(t)$ is norm bounded on $[0, T)$. Thus, by Theorem X.74, global solutions exist.
(e) Check that the proofs of smoothness and propagation speed one go through as in the case of positive mass.

†77. Prove that

$$\int h\{f, g\}\, dx = \int \{h, f\} g\, dx$$

for any $f, g, h \in C_0^1(\mathbb{R}^{6N})$.

†78. Prove the proposition before Theorem X.78.

79. Let $C_{0,\infty}(\mathbb{R})$ denote the continuous functions vanishing at 0 and ∞. Let $D = d/dx$. Prove that D and $-D$ on the natural domain are accretive, but only one of them generates a contraction semigroup.

80. Let A, J, and $\mathscr{H}$ satisfy the hypothesis of Theorem X.74 (except that J is not required to satisfy the hypothesis of part (b) of Theorem X.73). Suppose that for all k, the solutions of (X.143) are a priori bounded uniformly for all $\|\varphi(0)\| \leq k$. Prove that for each $j = 0, 1, \ldots, n$, and each k, there is a monotone increasing (everywhere finite) function $d_{j,k}(\cdot)$ on $(0, \infty)$ so that

$$\|A^j\varphi_1(t) - A^j\varphi_2(t)\| \leq d_{j,k}(|t|)\|\varphi_1(0) - \varphi_2(0)\|$$

for all solutions φ_i of (X.143) with $\|\varphi_i(0)\| \leq k$. Hint: Use the idea of Theorem X.75 and the trick of Lemma 1.

81. Let C be a complex conjugation on a Hilbert space $\mathscr{H}$. Let A be a symmetric operator with $C : D(A) \to D(A)$ and $AC = CA$. An extension B of A is called real if $C : D(B) \to D(B)$ and $BC = CB$.
(a) Let $\{\varphi_n\}_{n=1}^N$ be an orthonormal basis for $\mathscr{K}_+$, the deficiency space for A. Define $J : \mathscr{K}_+ \to \mathscr{K}_+$ by $J(\sum a_n\varphi_n) = \sum \bar{a}_n\varphi_n$. If U is a unitary operator from $\mathscr{K}_+$ to $\mathscr{K}_-$, prove that the associated self-adjoint extension A_U is real if and only if $JCU : \mathscr{K}_+ \to \mathscr{K}_+$ has a matrix w.r.t. $\{\varphi_n\}$ which is its own transpose.
(b) Prove that A always has real self-adjoint extensions.
(c) If A has deficiency indices 1, prove that every self-adjoint extension is real. Verify this in the example $-d^2/dx^2$ on $C_0^\infty(0, \infty) \subset L^2(0, \infty)$.
(d) If A has deficiency indices 2 or more, prove that A has self-adjoint extensions which are not real. Verify this in the example $-d^2/dx^2$ on $C_0^\infty(0, 1) \subset L^2(0, 1)$.

READER'S GUIDE

In this chapter, we develop techniques for proving the existence of solutions of the basic dynamical equations in a wide variety of physical situations. We emphasize the applications to quantum mechanics and quantum field theory, and in these cases the existence of dynamics is "equivalent" to proving that the Hamiltonian is self-adjoint. Thus, these techniques are mainly

methods of proving that a given operator is self-adjoint. The following table lists the sections where various physical operators are proven self-adjoint:

	Sections
Atomic Hamiltonians	2
Stark effect Hamiltonians	5, 1 (Appendix) for the one-dimensional case
Zeeman effect Hamiltonians	4
Anharmonic oscillator	2, 4, 6, 9, 10
Quantum field Hamiltonians	7, 9
Quantum field operators	5, 6, 7

It is not necessary for the reader to know all the material in Chapter IX before studying Chapter X. He should, however, know the basic properties of the Fourier transform presented in Sections IX.1 and IX.2 and the properties of the free Hamiltonian discussed in Section IX.7 since this material is used throughout Chapter X without comment. Other theorems about the Fourier transform (for example, the Paley-Wiener theorems and the interpolation theorems) are also used, but the reader can easily refer back to Chapter IX when necessary.

We give a section by section description of Chapter X below; here is a summary. The fundamental properties of self-adjoint operators are discussed in Section VIII.3 and Sections X.1 and X.2. The reader interested in quantum mechanics should know in addition the material in Section VIII.11 and Sections 1 (Appendix), 2, 3, 4, 5, 11, and 12 of Chapter X. The basic discussions of quantum field theory are given in Section IX.8 and Section X.7. The reader interested in quantum field theory should also know the mathematical techniques in Sections 5, 6, 9, 10, and 11 of Chapter X. Self-adjointness techniques can be used to prove the existence and regularity of solutions for certain types of partial differential equations. Such applications appear in Sections 3, 8, 12, and 13 of Chapter X. The Appendix to Section 1 contains applications to ordinary differential equations.

In Section 1 we describe the closed symmetric extensions of symmetric operators by using the theory of deficiency indices. We also prove von Neumann's theorem that a symmetric operator which commutes with a conjugation has self-adjoint extensions. In the Appendix to Section 1 we discuss Weyl's limit point–limit circle criteria and compare the quantum and classical motions on a half-line.

In Section 2 we prove the Kato–Rellich theorem on small perturbations of self-adjoint operators and the KLMN theorem on small form perturbations. The Kato–Rellich theorem is then used to prove the self-adjointness of atomic Hamiltonians.

In Sections 3 and 4 we apply two distinct notions of positivity. In Section 3 we study positive quadratic forms and discuss properties of the Friedrichs extension. In Section 4 we prove a distribution inequality of Kato and use it to show that $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ if V is locally L^2 and bounded below. This technique is then used to prove the self-adjointness of the Zeeman effect Hamiltonian.

In Section 5 we show that if A is dominated by a strictly positive operator N and $[A, N]$ is suitably small, then A is essentially self-adjoint on any core for N. This result is then applied to prove the self-adjointness of the Stark effect Hamiltonian.

In Section 6 we prove Nelson's analytic vector criterion for self-adjointness.

In Section 7 we define the free scalar hermitian Bose field of mass $m > 0$ and prove that it satisfies the Gårding–Wightman axioms. This section should be read in conjunction with Section IX.8. We also introduce Q space and the spatially cut-off Hamiltonian for the $(\varphi^4)_2$

field theory. In the Appendix, we prove that for different m, the free scalar Hermitian field gives rise to inequivalent representations of the canonical commutation relations.

In Section 8 we discuss the natural generalization of many of these self-adjointness techniques to Banach spaces. We characterize the generators of contraction semigroups (the Hille–Yosida and Lumer–Phillips theorems) and introduce holomorphic semigroups. The techniques are used to prove various properties of the solution of the heat equation.

In Section 9 we discuss a special class of semigroups, hypercontractive semigroups, and prove the essential self-adjointness of the spatially cut-off Hamiltonian for the $(\varphi^4)_2$ quantum field theory.

In Section 10 we continue the discussion of graph limit methods for proving self-adjointness begun in Section VIII.7.

In Section 11 we discuss Feynman path integrals, integration on function space, and prove the Feynman–Kac formula.

In Section 12 we prove the existence of solutions of the equation $U'(t) = -A(t)U(t)$ when $A(t)$ is a suitable family of operators on a Banach space. We apply the result to solve the Schrödinger equation with time-dependent potentials and the heat equation with time-dependent sources and sinks.

In Section 13, we prove the existence, smoothness, and finite propagation speed for the nonlinear equation $(\Box^2 + m^2)u = -\lambda u^3$.

In Section 14 we very briefly describe the reformulation of classical mechanics as a Hilbert space problem.

List of Symbols

Page numbers in italics refer to Volume I.

$A, A^{\dagger}, A^{\#}$ *142*, 204
$a(\cdot), a^{-}(\cdot), a^{\dagger}(\cdot)$ (annihilation and creation operators) 208, 217–219
$AC[0, 1]$ *254*
$a(x, \theta)$ 99
$\mathbb{C}$ the complex numbers
$C(X)$ *102*
$C_{\mathbb{R}}(X)$ *101*, *102*
$C_{\infty}(\mathbb{R}^n)$ *111*, 10, 243
$C_0^{\infty}(\mathbb{R}^n)$ *145*
$C^{\infty}(A)$ 201
$d\Gamma(A)$ *302*, 208
$D(\cdot)$ (domain) *249*
$\mathscr{D}(\mathbb{R}^n), \mathscr{D}(\Omega)$ *147*
$\mathscr{D}'(\mathbb{R}), \mathscr{D}'(\Omega)$ *148*
D^{α} 2
$D_{\mathscr{S}}$ 218
$f(A)$ (continuous functional calculus) *222*
$\hat{f}, \mathscr{F}$ (Fourier transform) 1
$\check{f}, \mathscr{F}^{-1}$ (inverse Fourier transform) 1
$\hat{f}$ (Section X.7 only) 212
$\mathscr{F}_M$ 76
$\mathscr{F}(\mathscr{H}), \mathscr{F}_s(\mathscr{H}), \mathscr{F}_s(\mathscr{H})$ *53*, *54*, 207
F_0 208
$G_0(x, y; E)$ free Green's function) 59
$\mathscr{H}$ *39*
$\mathscr{H}_{pp}, \mathscr{H}_{ac}, \mathscr{H}_{sing}$ *230*
$\mathscr{H}_C$ 215
$\mathscr{H}^{(n)}, \mathscr{H}_s^{(n)}$ (*n*-particle subspace) 207–208
$H(g)$ 227
H_0 (free Hamiltonian) 55
H_m (mass hyperboloid) 70
$\mathscr{I}_p$ *207*, *208*, 41
$I(U)$ (initial space) *197*
Ker *185*
KLMN 167
ℓ_2 *40*
ℓ_p *69*
ℓ_{∞} *69*
L^1 *17*
L^2 *39*
L^{∞} *67*
$L^p(X, d\mu)$ *68*
$L^2(X, d\mu; \mathscr{H}')$ *40*
$L^p(M, d\mu; E)$ *89*
$L^2(Q, d\mu)$ (Q-space) 228
L^p_{loc} (functions locally L^p) 353
$L^2_{\mathbb{R}}(X)$ (real-valued functions) 353
L^2_m (weighted L^2) 76
L^p_w (weak L^p) 30
$L^r + L^s$ 165
$\mathscr{L}, \mathscr{L}^1_+$ 63
$\mathscr{L}_+(\mathbb{C})$ 68

$\mathscr{L}(\mathscr{H})$		*182*
$\mathscr{L}(X, Y)$		*69*
$\mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$		192
$M(\varphi)$		101
$\mathscr{M}(X), \mathscr{M}_+(X), \mathscr{M}_{+,1}(X)$		*109*
$n_\pm(A)$		138
N	(number operator)	*142*, 204, 208, 220
O_M^n		*137*
$P_\Omega(A), P_\Omega^A$		*234*
$p(D)$		45
$\mathscr{P}, \mathscr{P}_+^\uparrow$		63
$Q(q), Q(A)$		*276*, *277*
Q-space		228
$\mathbb{R}$		the real numbers
$\mathbb{R} - iC$	(tube with base C)	19
$R_\lambda(T)$	(resolvent)	*188*
Ran		*185*
sing supp		88
supp		*139*, 17
$SP(\varphi)$		101
Sym(Ω, s, m)		99
$\mathscr{S}(\mathbb{R}^n)$		*133*
$\mathscr{S}'(\mathbb{R}^n)$		*134*
$\mathscr{S}_\mathbb{R}(\mathbb{R}^n)$	(real-valued functions)	354
Tr($\cdot$)		*207*, *208*
$\mathscr{T}_n, \mathscr{T}_n^c$		66, 68
V_+		63
$W_m(\Omega)$	(Sobolev space)	50
$W_n, \mathscr{W}_n$	(Wightman function)	66
$WF(T), WF_x(T)$		92
x^α		2

$\Gamma(T)$	(graph)	*250*
$\Gamma(A)$		*309*, 208
$d\Gamma(A)$		*302*, 208
$\Gamma_{a,\theta}, \Gamma_{a,\theta}^*$		19
$\Delta_+(x; m^2)$		71
$\mu(p)$		216
μ_ψ		*225*
$\pi(f)$		215
$\pi_m(f)$		216
$\rho(T)$		*188*
$\sigma(T)$		*188*
$\sigma_{pp}, \sigma_{cont}, \sigma_{ac}, \sigma_{sing}$		*231*
$\sigma_{disc}, \sigma_{ess}$		*236*
$\varphi(f)$	(Wightman field)	64
$\varphi(f)$	(Canonical free field)	215
$\varphi_m(f)$		216
$\Phi_S(f)$		209
$\Phi_m(f)$		212
ϕ_n	(Hermite functions)	*143*, 204
χ_A		*2*
ψ_0	(vacuum)	63
Ω_0	(vacuum)	208
Ω_m	(mass hyperboloid)	70

$\|\cdot\|_1$		*9*
$\|\cdot\|_\infty$		*9*
$\|\cdot\|_{\alpha,\beta}$		*133*
$\|\cdot\|_{\alpha,\beta,2}$, $\|\cdot\|_{\alpha,\beta,\infty}$		141

$\oplus$		*40*, *78*
$\otimes$	(measures)	*26*
$\otimes$	(Hilbert spaces)	*49*
$\otimes$	(functions)	*141*
$\otimes$	(operators)	*299*

$<<$	infinitesimally small (operators)	162
$\prec\prec$	infinitesimally small forms	168
$-$	(closure)	*92*
$\circ$	(interior)	*92*
$*$	(adjoint)	*187*
$*$	(dual space)	*72*
$*$	convolution	6, 7
$\xrightarrow{\|\cdot\|}$, $\xrightarrow{w}$, $\xrightarrow{s}$		*182*, *183*
$\|\cdot\|$	(absolute value of an operator)	*196*
$^\perp$	(orthogonal complement)	*41*
$\setminus$	(set difference)	*1*
$/$	(quotient)	*78*, *79*
$\restriction$	(restriction)	*2*
$\langle\cdot,\cdot\rangle$	(ordered pair)	*1*
$(\cdot,\cdot)$	(inner product)	*36*
$\{\cdot,\cdot\}$	(Poisson bracket)	314

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METHODS OF MODERN MATHEMATICAL PHYSICS

III: SCATTERING THEORY

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To Martha and Jackie

Introduction

Scattering theory is the study of an interacting system on a scale of time and/or distance which is large compared to the scale of the interaction itself. As such, it is the most effective means, sometimes the only means, to study microscopic nature. To understand the importance of scattering theory, consider the variety of ways in which it arises. First, there are various phenomena in nature (like the blue of the sky) which are the result of scattering. In order to understand the phenomenon (and to identify it as the result of scattering) one must understand the underlying dynamics and its scattering theory. Second, one often wants to use the scattering of waves or particles whose dynamics one knows to determine the structure and position of small or inaccessible objects. For example, in x-ray crystallography (which led to the discovery of DNA), tomography, and the detection of underwater objects by sonar, the underlying dynamics is well understood. What one would like to construct are correspondences that link, via the dynamics, the position, shape, and internal structure of the object to the scattering data. Ideally, the correspondence should be an explicit formula which allows one to reconstruct, at least approximately, the object from the scattering data. A third use of scattering theory is as a probe of dynamics itself. In elementary particle physics, the underlying dynamics is not well understood and essentially all the experimental data are scattering data. The main test of any proposed particle dynamics is whether one can construct for the dynamics a scattering theory that predicts the observed experimental data. Scattering theory was not always so central to physics. Even though the Coulomb cross section could have been computed by Newton, had he bothered to ask the right question, its calculation is generally attributed to Rutherford more than two hundred years later. Of course, Rutherford's calculation was in connection with the first experiment in nuclear physics.

Scattering theory is so important for atomic, condensed matter, and high

energy physics that an enormous physics literature has grown up. Unfortunately, the development of the associated mathematics has been much slower. This is partially because the mathematical problems are hard but also because lack of communication often made it difficult for mathematicians to appreciate the many beautiful and challenging problems in scattering theory. The physics literature, on the other hand, is not entirely satisfactory because of the many heuristic formulas and ad hoc methods. Much of the physics literature deals with the "time-independent" approach to scattering theory because the time-independent approach provides powerful calculational tools. We feel that to use the time-independent formulas one must understand them in terms of and derive them from the underlying dynamics. Therefore, in this book we emphasize scattering theory as a time-dependent phenomenon, in particular, as a comparison between the interacting and free dynamics. This approach leads to a certain imbalance in our presentation since we therefore emphasize large times rather than large distances. However, as the reader will see, there is considerable geometry lurking in the background.

The scattering theories in branches of physics as different as classical mechanics, continuum mechanics, and quantum mechanics, have in common the two foundational questions of the existence and completeness of the wave operators. These two questions are, therefore, our main object of study in individual systems and are the unifying theme that runs throughout the book. Because we treat so many different systems, we do not carry the analysis much beyond the construction and completeness of the wave operators, except in two-body quantum scattering, which we develop in some detail. However, even there, we have not been able to include such important topics as Regge theory, inverse scattering, and double dispersion relations.

Since quantum mechanics is a linear theory, it is not surprising that the heart of the mathematical techniques is the spectral analysis of Hamiltonians. Bound states (corresponding to point spectra) of the interaction Hamiltonian do not scatter, while states from the absolutely continuous spectrum do. The mathematical property that distinguishes these two cases (and that connects the physical intuition with the mathematical formulation) is the decay of the Fourier transform of the corresponding spectral measures. The case of singular continuous spectrum lies between and the crucial (and often hardest) step in most proofs of asymptotic completeness is the proof that the interacting Hamiltonian has no singular continuous spectrum. Conversely, one of the best ways of showing that a self-adjoint operator has no singular continuous spectrum is to show that it is the interaction Hamiltonian of a quantum system with complete wave operators. This deep

connection between scattering theory and spectral analysis shows the artificiality of the division of material into Volumes III and IV. We have, therefore, preprinted at the end of this volume three sections on the absence of continuous singular spectrum from Volume IV.

While we were reading the galley proofs for this volume, V. Enss introduced new and beautiful methods into the study of quantum-mechanical scattering. Enss's paper is not only of interest for what it proves, but also for the future direction that it suggests. In particular, it seems likely that the methods will provide strong results in the theory of multiparticle scattering. We have added a section at the end of this Chapter (Section XI.17) to describe Enss's method in the two-body case. We would like to thank Professor Enss for his generous attitude, which helped us to include this material.

The general remarks about notes and problems made in earlier introductions are applicable here with one addition: the bulk of the material presented in this volume is from advanced research literature, so many of the problems are quite substantial. Some of the starred problems summarize the contents of research papers!

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XI: Scattering Theory

It is notoriously difficult to obtain reliable results for quantum mechanical scattering problems. Since they involve complicated interference phenomena of waves, any simple uncontrolled approximation is not worth more than the weather forecast. However, for two body problems with central forces the computer can be used to calculate the phase shifts . . . . *W. Thirring*

XI.1 An overview of scattering phenomena

In this chapter we shall discuss scattering in a variety of physical situations. Our main goal is to illustrate the underlying similarities between the large time behavior of many kinds of dynamical systems. We study the case of nonrelativistic quantum scattering in great detail. Other systems we treat to a lesser extent, emphasizing simple examples.

Scattering normally involves a comparison of two different dynamics for the same system: the given dynamics and a "free" dynamics. It is hard to give a precise definition of "free dynamics" which will cover all the cases we consider, although we shall give explicit definitions in each individual case. The characteristics that these free dynamical systems have in common are that they are simpler than the given dynamics and generally they conserve the momentum of the "individual constituents" of the physical system. It is important to bear in mind that scattering involves more than just the interacting dynamics since certain features of the results will seem strange otherwise. Because two dynamics are involved, scattering theory can be viewed as a branch of perturbation theory. In the quantum-mechanical case we shall see that the perturbation theory of the absolutely continuous spectrum is

involved rather than the perturbation theory of the discrete spectrum discussed in Chapter XII.

Scattering as a perturbative phenomenon emphasizes temporal asymptotics, and this is the approach we shall generally follow. But all the *concrete* examples we discuss will also have a geometric structure present and there is clearly lurking in the background a theory of scattering as correlations between spatial and temporal asymptotics. This is an approach we shall not explicitly develop, in part because it has been discussed to a much lesser degree. We do note that all the "free" dynamics we discuss have "straight-line motion" in the sense that solutions of the free equations which are concentrated as $t \to -\infty$ in some neighborhood of the direction $\mathbf{n}$ are concentrated as $t \to +\infty$ in a neighborhood of the direction $-\mathbf{n}$. These geometric ideas are useful for understanding the choice of free dynamics in Sections 14 and 16 where a piece of the interacting dynamics generates the free dynamics. And clearly, the geometric ideas are brought to the fore in the Lax–Phillips theory (Section 11) and in Enss's method (Section 17).

Scattering theory involves studying certain states of an interacting system, namely those states that appear to be "asymptotically free" in the distant past and/or the distant future. To be explicit, suppose that we can view the dynamics as transformations acting on the states. Let T_t and $T_t^{(0)}$ stand for the interacting and free dynamical transformations on the "set of states" Σ. Σ may be points in a phase space (classical mechanics), vectors in a Hilbert space (quantum mechanics), or Cauchy data for some partial differential equation (acoustics, optics). One is interested in pairs $\langle \rho_-, \rho \rangle \in \Sigma$ so that

$$\lim_{t \to -\infty} (T_t \rho - T_t^{(0)} \rho_-) = 0$$

for some appropriate sense of limit, and similarly for pairs that approach each other as $t \to +\infty$. One requirement that one must make on the notion of limit is that for each ρ there should be at most one ρ_-.

The basic questions of scattering theory are the following:

(1) *Existence of scattering states* Physically, one prepares the interacting system in such a way that some of the constituents are so far from one another that the interaction between them is negligible. One then "lets go," that is, allows the interacting dynamics to act for a long time and then looks at what has happened. One usually describes the initial state in terms of the variables natural to describe free states, often momenta. One expects that any free state "can be prepared," that is, for any $\rho_- \in \Sigma$, there is a $\rho \in \Sigma$ with $\lim_{t \to -\infty} T_t \rho - T_t^{(0)} \rho_- = 0$. Proving this is the basic existence question of scattering.

(2) *Uniqueness of scattering states* In order to describe the prepared state in terms of free states, one must know that each free state is associated with a unique interacting state; that is, given ρ_- there is at most one ρ such that $T_t^{(0)} \rho_- - T_t \rho \to 0$ as $t \to -\infty$. Notice that this is distinct from the requirement on the limit above that there should be at most one ρ_- for each ρ.

(3) *Weak asymptotic completeness* Suppose that one has an interacting state ρ that looked like a free state in the distant past in the sense that $\lim_{t \to -\infty} T_t^{(0)} \rho_- - T_t \rho = 0$ for some state ρ_-. One hopes that for large positive times, the interacting state will again look like a free state in the sense that there exists a state ρ_+ so that $\lim_{t \to +\infty} T_t^{(0)} \rho_+ - T_t \rho = 0$. In order to prove this, one needs to show that the two subsets of Σ

$$\Sigma_{\text{in}} = \left\{ \rho \in \Sigma \,\middle|\, \exists \rho_- \in \Sigma \text{ with } \lim_{t \to -\infty} T_t^{(0)} \rho_- - T_t \rho = 0 \right\}$$

and

$$\Sigma_{\text{out}} = \left\{ \rho \in \Sigma \,\middle|\, \exists \rho_+ \in \Sigma \text{ with } \lim_{t \to +\infty} T_t^{(0)} \rho_+ - T_t \rho = 0 \right\}$$

are equal. If in fact $\Sigma_{\text{in}} = \Sigma_{\text{out}}$, then the system is said to have **weak asymptotic completeness.**

(4) *Definition of the S-transformation* If one has a pair of dynamical systems $\langle T_t^{(0)}, T_t \rangle$ for which one can prove existence and uniqueness of scattering states (both as $t \to -\infty$ and as $t \to \infty$) and for which weak asymptotic completeness holds, then one can define a natural bijection of Σ onto itself. Given $\rho \in \Sigma$, existence and uniqueness of scattering states assures us that there exists a state $\Omega^+ \rho \in \Sigma_{\text{in}}$ with $\lim_{t \to -\infty} (T_t(\Omega^+ \rho) - T_t^{(0)} \rho) = 0$. Similarly, Ω^- is defined by $\lim_{t \to +\infty} (T_t(\Omega^- \rho) - T_t^{(0)} \rho) = 0$. Ω^+ (respectively, Ω^-) is a bijection from Σ onto Σ_{in} (respectively, Σ_{out}). Weak asymptotic completeness assures us that $\Sigma_{\text{in}} = \Sigma_{\text{out}}$, so one can define the *bijection*

$$S = (\Omega^-)^{-1} \Omega^+ : \Sigma \to \Sigma$$

S is called the **scattering transformation.** Thus, $T_t^{(0)}(S\rho)$ and $T_t^{(0)} \rho$ are related by the condition that there exists a state ψ ($\psi = \Omega^+ \rho = \Omega^-(S\rho)$) so that $T_t \psi$ "interpolates" between them. That is, $T_t \psi$ looks like $T_t^{(0)} \rho$ in the past and $T_t^{(0)} S\rho$ in the future. Thus S correlates the past and future asymptotics of interacting histories. The reader should be warned that the maps $S' = \Omega^+ (\Omega^-)^{-1} : \Sigma_{\text{in}} \to \Sigma_{\text{out}}$ and also the maps $(\Omega^+)^{-1} \Omega^-$ and $\Omega^- (\Omega^+)^{-1}$ occasionally appear in the literature. When weak asymptotic completeness holds, $S' = \Omega^- S (\Omega^-)^{-1}$, so S and S' are "similar." For this reason, the choice between S and S' is to some extent a matter of personal preference. We use S,

the so-called EBFM S-matrix, throughout this book. We discuss the reasons for the $\pm$ convention in Sections 3 and 6.

In classical particle mechanics S is a bijection on phase space. In a quantum theory with weak asymptotic completeness S is a *linear* unitary transformation and is called the S-operator or occasionally the S-matrix.

(5) *Reduction of S due to symmetries* In many problems there is an underlying symmetry of *both* the free and interacting dynamics. This allows one to conclude a priori, without detailed dynamical calculations, that S has a special form. See Sections 2 and 8 for explicit details.

(6) *Analyticity and the S-transformation* A common refinement of scattering theory for wave phenomena (quantum theory, optics, acoustics) is the realization of S or the kernel of some associated integral operator as the boundary value of an analytic function. In a heuristic sense this analyticity is connected with Theorem IX.16. For schematically, S describes the response R of a system to some input I in the following form:

$$R(t) = \int_{-\infty}^{t} f(t - t')I(t')\, dt'$$

This formula has two features built in: (i) time translation invariance, that is, f is a function of only $t - t'$; (ii) causality: $R(t)$ depends only on $I(t')$ for $t' \leq t$. Thus f is a function on $[0, \infty)$. Its Fourier transform is thus the boundary value of an analytic function. It is this causality argument that is intuitively in the back of physicists' minds when discussing analytic properties. Unfortunately, the proofs of these properties do not go along such simple lines. We shall restrict our detailed discussion of analyticity to the two-body quantum-mechanical case (Section 7) and to the Lax-Phillips theory (Section 11).

(7) *Asymptotic completeness* Consider a system with forces between its components that fall off as the components are moved apart. Physically, one expects a state of such a system to "decay" into freely moving clusters or to remain "bound." In many situations, there is a natural set of bound states, $\Sigma_{\text{bound}} \subset \Sigma$. One can usually prove that $\Sigma_{\text{bound}} \cap \Sigma_{\text{in}} = \varnothing$. The above physical expectation is

$$\Sigma_{\text{bound}} \text{ "+" } \Sigma_{\text{in}} = \Sigma = \Sigma_{\text{bound}} \text{ "+" } \Sigma_{\text{out}} \tag{1}$$

" + " is different in classical and quantum-mechanical systems. In classical particle mechanics " + " indicates set theoretic union; in quantum theory it indicates a direct sum of Hilbert spaces. Establishing that (1) holds is the problem of proving **asymptotic completeness**. Notice that asymptotic completeness implies weak asymptotic completeness. We remark that implicit in the idea that each free state has an associated interacting state is the assumption that the free dynamics has no "bound" states.

We emphasize that the above description is schematic. In each physical theory there are complications, and various modifications must be made. Among these are: (i) In classical mechanics Σ comes equipped with sets of measure zero and the natural interpretation of statements like $\Sigma_{\text{in}} = \Sigma_{\text{out}}$ is that they differ by sets of measure zero. (ii) In some systems, including many-body systems, the state spaces of the free and interacting dynamics are different (see Sections 5, 15, and 16). (iii) In quantum-mechanical systems one can define an S-operator even without weak asymptotic completeness (see Section 4). Weak asymptotic completeness then becomes equivalent to the unitarity of S. (iv) In certain very special cases the free dynamics may have bound states (see Section 10). (v) In the Lax-Phillips theory (Section 11) the free dynamics is replaced by the geometric notion of "incoming" and "outgoing" subspaces.

Usually, the interacting dynamics is obtained initially by perturbing a simple dynamics which then plays the role of the "free" dynamics. However, in some special physical theories there is no natural unperturbed dynamics to compare with the interacting dynamics. In such cases one first isolates certain especially simple solutions of the interacting system. Then one tries to describe the asymptotic behavior of the complete interacting system in terms of the interactions of these simple solutions. Magnon scattering (Section 14) and the Haag-Ruelle theory (Section 16) are examples of such systems, as is the scattering theory for the Korteweg-deVries equation, which we do not treat.

XI.2 Classical particle scattering

The simplest system with which to illustrate the ideas of scattering theory is the classical mechanics of a single particle moving in an external force field $\mathbf{F}(\mathbf{r})$. This theory is equivalent to the scattering of two particles interacting with each other through a force field $\mathbf{F}(\mathbf{r}_1 - \mathbf{r}_2)$ because the center of mass motion of such a two-body system separates from the motion of $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$. We shall suppose that the particle has mass one, which is no loss of generality.

The states of such a single particle system are points in **phase space**, that is, a pair $\langle \mathbf{r}, \mathbf{v} \rangle \in \mathbb{R}^6$ representing the position and velocity of the particle. The free dynamical transformation is given by $T_t^{(0)}\langle \mathbf{r}, \mathbf{v} \rangle = \langle \mathbf{r} + \mathbf{v}t, \mathbf{v} \rangle$. Thus the

free dynamics conserves the velocity. The interacting dynamics is given by $T_t\langle \mathbf{r}_0, \mathbf{v}_0\rangle = \langle \mathbf{r}(t), \mathbf{v}(t)\rangle$ where $\mathbf{v}(t) = \dot{\mathbf{r}}(t)$ and $\mathbf{r}(t)$ solves the equation

$$\ddot{\mathbf{r}}(t) = \mathbf{F}(\mathbf{r}(t)) \tag{2a}$$

with initial conditions

$$\mathbf{r}(0) = \mathbf{r}_0, \qquad \dot{\mathbf{r}}(0) = \mathbf{v}_0 \tag{2b}$$

In order to be sure that (2) has a unique solution for all times, we shall suppose that

$$|\mathbf{F}(\mathbf{r})| \leq C \qquad \text{for all } \mathbf{r} \tag{3a}$$

$$|\mathbf{F}(\mathbf{r}) - \mathbf{F}(\mathbf{r}')| \leq D_R|\mathbf{r} - \mathbf{r}'| \qquad \text{if} \quad |\mathbf{r} - \mathbf{r}'| \leq 1 \quad \text{and} \quad |\mathbf{r}| < R \tag{3b}$$

where D_R is an R-dependent constant. The techniques we developed in Section V.6 assure us that (2) has a unique solution for small time if (3b) holds, and it is not hard to prove that this solution exists for all times (see Proposition 1 in the appendix to Section X.1 and Problem 1). The only place where the conditions (3) enter in the theory that we shall develop is in establishing this global existence and uniqueness. If one can establish this by some other means, (3) can be dispensed with and conditions (4) below need be required to hold only for large distances. In particular, local repulsive singularities present no problem.

To establish the existence and uniqueness of scattering solutions, we shall need to have further restrictions on the forces. These restrictions, which require that the interaction between constituents falls off as $r \to \infty$, where $r = |\mathbf{r}|$, are typical of scattering theories. Specifically, we shall suppose that:

$$|\mathbf{F}(\mathbf{r})| \leq Cr^{-\alpha} \qquad \text{for all } \mathbf{r} \text{ and some } \alpha > 2 \tag{4a}$$

$$|\mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{y})| \leq Dr^{-\beta}|\mathbf{x} - \mathbf{y}| \qquad \text{for all } \mathbf{x}, \mathbf{y} \text{ with } x, y \geq r \text{ and some } \beta > 2 \tag{4b}$$

Under these assumptions we shall prove the existence and uniqueness of scattering solutions. One can establish existence using only (4a) (Problem 2), but uniqueness requires the Lipschitz condition (4b) (Problem 3). This is reminiscent of the situation we encountered in Section V.6 when discussing solutions of differential equations with initial conditions. Lipschitz conditions were also required there for uniqueness. This is not surprising since according to our intuitive picture in Section 1, scattering solutions can be viewed as solutions obeying "initial conditions at $t = -\infty$."

The conditions (4) do not include the important case of Coulomb scattering where the theory must be modified. We discuss this case in Section 9.

Henceforth we shall drop the boldface notation for vectors except in the statements of theorems and in situations where confusion might arise between a vector and its length.

Theorem XI.1 (existence and uniqueness of scattering solutions; classical particles) Let $\mathbf{F}(\mathbf{r})$ be a function from $\mathbb{R}^3$ to $\mathbb{R}^3$ obeying (3) and (4). Let $\langle \mathbf{r}_{-\infty}, \mathbf{v}_{-\infty}\rangle \in \mathbb{R}^6$ be given with $\mathbf{v}_{-\infty} \neq 0$. Then there exists a unique solution of (2a) obeying

$$\lim_{t \to -\infty} |\dot{\mathbf{r}}(t) - \mathbf{v}_{-\infty}| = 0 \tag{5a}$$

and

$$\lim_{t \to -\infty} |\mathbf{r}(t) - \mathbf{r}_{-\infty} - \mathbf{v}_{-\infty} t| = 0 \tag{5b}$$

Proof Since we are assuming (3), by the above remarks it is sufficient to prove the existence and uniqueness of solutions in $(-\infty, T)$ for some T. In keeping with the idea that scattering solutions obey initial conditions at $t = -\infty$, it is natural to use the method of Section V.6.A and rewrite the differential equation as an integral equation. In fact, one can show (Problem 4) that $r(t)$ obeys (2a) and (5) on $(-\infty, T)$ if and only if $r(t) = r_{-\infty} + v_{-\infty} t + u(t)$, where u is continuous and satisfies

$$u(t) = \int_{-\infty}^{t} \int_{-\infty}^{s} F(r_{-\infty} + v_{-\infty}\tau + u(\tau))\, d\tau\, ds \tag{6}$$

where the integral converges absolutely.

Choose $T < 0$ so that:

(i) $|r_{-\infty} + v_{-\infty} t| \geq \frac{1}{2}|t|\,|v_{-\infty}|$ if $t < T$;
(ii) $C(\alpha - 1)^{-1}(\alpha - 2)^{-1}|\tfrac{1}{4}v_{-\infty}|^{-\alpha}|T|^{2-\alpha} < 1$;
(iii) $\gamma \equiv D(\beta - 1)^{-1}(\beta - 2)^{-1}|\tfrac{1}{4}v_{-\infty}|^{-\beta}|T|^{2-\beta} < 1$;
(iv) $\frac{1}{4}|T|\,|v_{-\infty}| > 1$.

Here C, α, D, β are the constants in condition (4). Now suppose that $u(t)$ is an $\mathbb{R}^3$-valued continuous function on $(-\infty, T)$ with $\|u\|_\infty \leq 1$. Let $r(t) = r_{-\infty} + v_{-\infty} t + u(t)$. (i) and (iv) assure us that $|r(t)| \geq \frac{1}{4}|t|\,|v_{-\infty}|$. By (4a), the integral $\int_{-\infty}^{t}\int_{-\infty}^{s} |F(r_{-\infty} + v_{-\infty}\tau + u(\tau))|\, d\tau\, ds$ converges absolutely.

Let

$$\mathscr{M}_T = \{u \in C(-\infty, T) \text{ with values in } \mathbb{R}^3 \mid \|u\|_\infty \leq 1\}$$

and define $\mathscr{F}: \mathscr{M}_T \to \mathscr{M}_T$ by

$$(\mathscr{F}u)(t) = \int_{-\infty}^{t} \int_{-\infty}^{s} F(r_{-\infty} + v_{-\infty}\tau + u(\tau))\, d\tau\, ds$$

(4a) and (ii) assure us that $\|\mathscr{F}u\|_\infty \le 1$ if $\|u\|_\infty \le 1$, so $\mathscr{F}$ maps the complete metric space $\mathscr{M}_T$ into itself. (4b) and (iii) imply that

$$\|\mathscr{F}u - \mathscr{F}v\|_\infty \le \gamma\|u - v\|_\infty$$

so $\mathscr{F}$ is a contraction on $\mathscr{M}_T$ since T was chosen to make $\gamma < 1$. Thus, by the contraction mapping principle (Theorem V.8), $\mathscr{F}$ has a unique fixed point in $\mathscr{M}_T$. It is easy to prove now that (6) has a unique solution. For if u_1 and u_2 both solve (6), then both will lie in $\mathscr{M}_{T'}$ for some $T' < T$. But by the above argument, there is a unique solution of (6) in $\mathscr{M}_{T'}$ for any $T' < T$, so $u_1 = u_2$ on $(-\infty, T')$. By the uniqueness of solutions with initial conditions at $-T' - 1$, $u_1 = u_2$ on $(-\infty, T)$. ∎

We now define two important maps:

Definition Let $\Sigma = \mathbb{R}^6$ and let $r_{a,b}^{(-\infty)}(t)$ be the solution of (2a) asymptotic to $a + bt$ at $-\infty$. Set $\Sigma_0 \equiv \Sigma\backslash\{\langle a, b\rangle | b = 0\}$. Then the **wave operator** $\Omega^+ : \Sigma_0 \to \Sigma$ is defined by

$$\Omega^+\langle a, b\rangle = \langle r_{a,b}^{(-\infty)}(0), \dot{r}_{a,b}^{(-\infty)}(0)\rangle$$

Similarly, Ω^- is defined by

$$\Omega^-\langle a, b\rangle = \langle r_{a,b}^{(+\infty)}(0), \dot{r}_{a,b}^{(+\infty)}(0)\rangle$$

Thus $\Omega^+ w$ is that point of phase space which is the $t = 0$ initial data for a solution of the interacting equations of motion which is asymptotic at $t = -\infty$ to the solution of the free equations of motion with data at $t = 0$ equal to w.

The wave operators have several important properties:

Theorem XI.2 Suppose that conditions (3) and (4) hold for a force field $\mathbf{F}(\mathbf{r})$ and let $\Omega^\pm$ be the associated wave operators. Then:

(a) Let T_t and $T_t^{(0)}$ be the interacting and free dynamics, respectively. Then for all $w \in \Sigma_0$,

$$\Omega^\pm w = \lim_{t \to \mp\infty} T_{-t} T_t^{(0)} w$$

where the limits are uniform on compact subsets of Σ_0.

(b) $\Omega^\pm T_s^{(0)} = T_s \Omega^\pm$ on Σ_0 for all s.

(c) (isometry of $\Omega^\pm$) If $\mathbf{F}$ is conservative, that is, if $\mathbf{F} = -\nabla V$ for some function V, then $\Omega^\pm$ are measure-preserving transformations.

(d) If $\mathbf{F}$ is conservative and $V(\mathbf{r}) \to 0$ as $r \to \infty$, then $E(\Omega^\pm w) = E_0(w)$ where $E(\mathbf{r}, \mathbf{v}) = \frac{1}{2}v^2 + V(\mathbf{r})$ and $E_0(\mathbf{r}, \mathbf{v}) = \frac{1}{2}v^2$.

(e) If $\mathbf{F}$ is C^∞ and

$$\left| \frac{\partial^{|\alpha|} F(\mathbf{r})}{\partial r_1^{\alpha_1} \cdots \partial r_3^{\alpha_3}} \right| \le D_\alpha r^{-|\alpha| - 2 - \varepsilon}$$

for all $\mathbf{r}$, α and some $\varepsilon > 0$, then $\Omega^\pm$ are C^∞ maps.

Proof (a) This is a typical property of $\Omega^\pm$ and will be used to define the analogues of $\Omega^\pm$ in quantum-mechanical situations. Since $\Omega^+ x = y$ means that $\lim_{t \to -\infty} |T_t y - T_t^{(0)} x| = 0$ and $(T_t)^{-1} = T_{-t}$, (a) is intuitively expected. We shall prove the formula for Ω^+; the proof is essentially identical for Ω^-. For fixed $T \in \mathbb{R}$, define $\mathscr{M}_T$ as before. For $\langle \mathbf{a}, \mathbf{b}\rangle \in \Sigma_0$, $t \le T$, and $u \in \mathscr{M}_T$, define the function $\mathscr{F}_{a,b,T}^{(t)} u$ on $(-\infty, T)$ by

$$(\mathscr{F}_{a,b,T}^{(t)} u)(s) = \int_t^s \int_t^\sigma F(a + b\tau + u(\tau))\, d\tau\, d\sigma$$

Let $\mathscr{F}_{a,b,T}^{(-\infty)} u$ be of the same form with $t = -\infty$. One now proves the following three facts (Problems 5, 6):

(i) For any compact $K \subset \Sigma_0$, we can find $T < 0$ so that for $\langle a, b\rangle \in K$ and $t \in (-\infty, T)$, $\mathscr{F}_{a,b,T}^{(t)}$ takes $\mathscr{M}_T$ into itself and is a contraction. The constant γ in the equation $\|\mathscr{F}_{a,b,T}^{(t)} u - \mathscr{F}_{a,b,T}^{(t)} v\|_\infty \le \gamma\|u - v\|_\infty$ may be chosen, independently of $\langle a, b\rangle \in K$ and $t \in (-\infty, T)$, to be less than 1.

(ii) If K and T are as defined in (i), for any $u \in \mathscr{M}_T$, $\lim_{t \to -\infty} \mathscr{F}_{a,b,T}^{(t)} u = \mathscr{F}_{a,b,T}^{(-\infty)} u$. The convergence is uniform on $\mathscr{M}_T$ and K.

(iii) A general result about contractions: Suppose that F_n form a family of maps of a complete metric space to itself. If $\rho(F_n p, F_n q) \le c\rho(p, q)$ for all p, q, n and some $c < 1$, if $\lim_{n \to \infty} F_n p = F_\infty p$ for all p, and if p_n (respectively, p_∞) are the unique fixed points of F_n (respectively, F_∞), then $\lim_{n \to \infty} p_n = p_\infty$. Moreover, the rate at which p_n converges to p_∞ depends only on the rate at which $F_n p_\infty$ converges to $F_\infty p_\infty = p_\infty$ and c.

Let $u_{a,b,T}^{(t)}$ be the fixed point of $\mathscr{F}_{a,b,T}^{(t)}$. We conclude that $\lim_{t \to -\infty} u_{a,b,T}^{(t)} = u_{a,b,T}^{(-\infty)}$. Now, using the fact that T_{-T+1} is continuous from

Σ to Σ, we conclude the proof of (a):

$$\begin{aligned}\Omega^+\langle a, b\rangle &= T_{-T+1}\langle a + b(T-1) + u^{(-\infty)}_{a,b,T}(T-1),\ b + \dot{u}^{(-\infty)}_{a,b,T}(T-1)\rangle \\ &= \lim_{t\to-\infty} T_{-T+1}\langle a + b(T-1) + u^{(t)}_{a,b,T}(T-1),\ b + \dot{u}^{(t)}_{a,b,T}(T-1)\rangle \\ &= \lim_{t\to-\infty} T_{-T+1}T_{-t+T-1}T^{(0)}_t\langle a, b\rangle \\ &= \lim_{t\to-\infty} T_{-t}T^{(0)}_t\langle a, b\rangle\end{aligned}$$

(b) This is a general consequence of (a) since

$$\Omega^\pm T^{(0)}_s w = \lim_{t\to\mp\infty} T_{-t}T^{(0)}_{s+t}w = \lim_{\tau\to\mp\infty} T_{-\tau+s}T^{(0)}_\tau w = T_s\Omega^\pm w$$

Here we have used the continuity of T_s and the fact that as $t\to\pm\infty, \tau = s + t\to\pm\infty$ for fixed s.

(c) This is another general feature of scattering theory which we shall meet in quantum scattering in a slightly different guise. For conservative systems, it is known that T_t is measure-preserving (Theorem X.78). Similarly, $T^{(0)}_t$ is measure-preserving, so $T_{-t}T^{(0)}_t$ is measure-preserving for all t. Let f be a continuous function of compact support on Σ_0. Then, by (a),

$$\int f(\Omega^+ w)\, d^6w = \lim_{t\to-\infty}\int f(T_{-t}T^{(0)}_t w)\, d^6w = \int f(w)\, d^6w$$

Thus Ω^+, and similarly Ω^-, are measure-preserving maps.

(d) Follows from (a), the conservation of energy ($E\circ T_t = E$) and the assumption that $V\to 0$ as $r\to\infty$.

(e) Under the hypothesis, $\mathscr{F}^{(-\infty)}_{a,b,T}u$ is a C^∞ map of $\Sigma_0\times\mathscr{M}_T$ into $\mathscr{M}_T$ (Problem 7). By a general theorem on smoothness of fixed points of contractions (Problem 5b) the fixed points of $\mathscr{F}^{(-\infty)}_{a,b,T}$ and hence their values at $t = T-1$ are C^∞. Since T_t is a C^∞ mapping for each t, propagating the solution from $t = T-1$ to $t = 0$, we conclude that $\Omega^\pm$ are C^∞ maps. ∎

The domains of $\Omega^\pm$ are all of Σ minus a set of measure 0. In general, the range of $\Omega^\pm$ will not be all of Σ or even Σ minus a set of measure zero.

Example Let F obey the hypotheses of (d) of Theorem XI.2. Then $\text{Ran}\,\Omega^+\subseteq\{\langle a', b'\rangle \mid \tfrac{1}{2}|b'|^2 + V(a') > 0\}$. The set

$$\{\langle a', b'\rangle \mid \tfrac{1}{2}|b'|^2 + V(a')\le 0\}$$

has nonzero measure if V is continuous and negative at any point.

Definition Let $\Sigma_{\text{in}} = \text{Ran}\,\Omega^+$, $\Sigma_{\text{out}} = \text{Ran}\,\Omega^-$, and let Σ_{bound} be the set of $\langle \mathbf{r}, \mathbf{v}\rangle$ so that the solution $\mathbf{r}(t)$ of (2) satisfies

$$\sup_t |\mathbf{r}(t)| + \sup_t |\dot{\mathbf{r}}(t)| < \infty$$

Thus, bound states are those whose trajectories lie in bounded regions of phase space. Weak asymptotic completeness says that $\Sigma_{\text{in}} = \Sigma_{\text{out}}$, and asymptotic completeness that $\Sigma_{\text{in}} = \Sigma_{\text{out}} = \Sigma\backslash\Sigma_{\text{bound}}$. Since we have already thrown out sets of measure zero (namely, $\{\langle a, b\rangle \mid b = 0\}$) in defining $\Omega^\pm$, we should be prepared to have these equalities modulo sets of measure zero. In general, there do exist solutions that are asymptotically free as $t\to-\infty$ but not as $t\to+\infty$ (capture; see Problem 9).

If the force is conservative, that is, $\mathbf{F}(r) = -\nabla V(\mathbf{r})$, then by our hypotheses on $\mathbf{F}$, V is smooth and bounded. In this case, by conservation of energy, $|\dot{\mathbf{r}}(t)|$ is automatically bounded, so $\langle r, v\rangle\in\Sigma_{\text{bound}}$ if and only if $\sup_t|\mathbf{r}(t)| < \infty$.

Theorem XI.3 (asymptotic completeness; two-body classical particle scattering) Let $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$ with $V\to 0$ as $r\to\infty$. Suppose also that $\mathbf{F}$ obeys (3) and (4). Then Σ_{in}, Σ_{out}, and $\Sigma\backslash\Sigma_{\text{bound}}$ agree up to sets of measure 0.

Proof Let $r_{q,v}(t)$ be the solution of $\ddot{r}(t) = F(r(t))$, $r(0) = q$, $\dot{r}(0) = v$. Define

$$N_\pm = \left\{\langle q, v\rangle \,\middle|\, \overline{\lim_{t\to\pm\infty}}\, |r_{q,v}(t)| < \infty\right\}$$

We first want to show that N_+ and N_- agree up to sets of measure 0, that is, $\mu(N_+\backslash N_-) + \mu(N_-\backslash N_+) = 0$ where μ is Lebesgue measure. The measurability of sets like N_+, N_-, Σ_{bound} is left to Problem 10. Let $\{K_n\}$ be compact subsets of $\mathbb{R}^6$ with $\bigcup K_n = \mathbb{R}^6$, $K_n\subset K^{\text{int}}_{n+1}$. Let $N^{(n)}_+ = \{\langle q, v\rangle \mid T_t\langle q, v\rangle\in K_n$ for all $t\in[0,\infty)\}$ and similarly for $N^{(n)}_-$. We first note that $N_\pm = \bigcup_n N^{(n)}_\pm$ for, using conservation of energy, if $\overline{\lim}_{t\to+\infty}|r_{q,v}(t)| < \infty$, then $T_t\langle q, v\rangle$ lies in a compact subset of $\mathbb{R}^6$ as t runs from 0 to ∞. Thus, if $p\in N_+\backslash N_-$, $p\in N^{(n)}_+\backslash N^{(n)}_-$ for some n. Therefore, it is sufficient to prove that $\mu(N^{(n)}_+\Delta N^{(n)}_-) = 0$ for each n. Let T_t be the interacting dynamics. We first note that $\bigcap_{k=1}^\infty T_k N^{(n)}_+\subset N^{(n)}_-$ and that $N^{(n)}_+\supset T_1 N^{(n)}_+\supset T_2 N^{(n)}_+\supset\cdots$. Thus

$$\mu(N^{(n)}_+\backslash N^{(n)}_-)\le\mu\left(N^{(n)}_+\Big\backslash\bigcap_{k=1}^\infty T_k N^{(n)}_+\right)\le\sum_{k=1}^\infty\mu(N^{(n)}_+\backslash T_k N^{(n)}_+)$$

But, by Liouville's theorem, $\mu(T_k N^{(n)}_+) = \mu(N^{(n)}_+) < \infty$. Since $T_k N^{(n)}_+\subset N^{(n)}_+$, we conclude that $\mu(N^{(n)}_+\backslash T_k N^{(n)}_+) = 0$, so $\mu(N^{(n)}_+\backslash N^{(n)}_-) = 0$. A similar proof shows that $\mu(N_-\backslash N_+) = 0$ so $\mu(N_+\,\Delta\, N_-) = 0$.

Now suppose $r(t)$ solves Newton's equation and $\overline{\lim}_{t\to\infty} |r(t)| = \infty$. We shall first show that if the energy $E(r(0), \dot{r}(0)) > 0$, then $|r(t)| \geq C|t|$ for t large and use this to prove that $r(t)$ approaches a free solution. Let $I(t) = \frac{1}{2}|r(t)|^2$ be the moment of inertia. Then

$$\dot{I}(t) = \dot{\mathbf{r}} \cdot \mathbf{r} = \dot{r}(t)r(t)$$

where $r(t) = |\mathbf{r}(t)|$ and $\dot{r}(t) = dr/dt$ (which is not equal to $|d\mathbf{r}/dt|$ in general). Also,

$$\begin{aligned}\ddot{I}(t) &= \dot{\mathbf{r}}(t)^2 + \mathbf{F}(\mathbf{r}(t)) \cdot \mathbf{r}(t) \\ &= 2E + \mathbf{r} \cdot \mathbf{F}(\mathbf{r}) - 2V(\mathbf{r})\end{aligned}$$

Since $E > 0$, and both $r \cdot F$ and V go to zero as $r \to \infty$, we can find R_0 so that $|r| > R_0$ implies $|r \cdot F(r) - 2V(r)| < E$. Since $\overline{\lim}_{t\to\infty} |r(t)| = \infty$, we can find some t_0 with $r(t_0) > R_0$, $\dot{r}(t_0) > 0$. We now claim that $r(t) > R_0$ for all $t > t_0$; for if not, let t_1 be the smallest $t > t_0$ with $r(t) = R_0$. Then $\ddot{I}(t) \geq E$ for $t \in [t_0, t_1]$ so that $\dot{I}(t_1) = r(t_1)\dot{r}(t_1) > \dot{I}(t_0) > 0$. Since $r(t) > R_0$ for $t = t_1 - \varepsilon$ and $r(t_1) = R_0$, we know that $\dot{r}(t_1) \leq 0$, and thus we have a contradiction. It follows that $r(t) > R_0$ for all $t > t_0$ and therefore for all $t > t_0$, $I(t) \geq a + bt + Et^2/2$ for suitable constants a and b. Thus $r(t) \geq \frac{1}{2}t\sqrt{E}$ for t sufficiently large. Using (4), we know that $\int_{t_0}^{\infty} F(r(t))\,dt$ exists, so we can define

$$b = \dot{r}(t_0) + \int_{t_0}^{\infty} F(r(t))\,dt = \lim_{t\to\infty} \dot{r}(t)$$

and

$$a = r(t_0) - bt_0 - \int_{t_0}^{\infty}\int_{s}^{\infty} F(r(t))\,dt\,ds = \lim_{t\to\infty}(r(t) - bt)$$

The second integral also exists. Moreover,

$$\lim_{t\to\infty} |r(t) - a - bt| + |\dot{r}(t) - b| = 0$$

Thus, if $E > 0$ and $\overline{\lim}_{t\to\infty} |r(t)| = \infty$, then $r(t)$ is a scattering solution, that is, $\langle r(0), \dot{r}(0)\rangle$ is in Σ_{out}.

Now, let Σ' be Σ with two sets of measure zero removed: namely, $N^+ \Delta N^-$, which has measure zero by the first part of our proof; and $\{\langle r, v\rangle | E(r, v) = 0\}$, which has measure zero since $\{v | E(r_0, v) = 0\}$ is a sphere that has measure zero for each fixed $\mathbf{r}_0$. Suppose that $w \in \Sigma'\backslash\Sigma_{\text{bound}}$ and let $r(t)$ be the solution of (2) with $\langle r(0), \dot{r}(0)\rangle = w$. Since $w \notin \Sigma_{\text{bound}}$, either $\lim_{t\to-\infty} |r(t)| = \infty$ or $\lim_{t\to+\infty} |r(t)| = \infty$ so $w \in (\Sigma\backslash N^+) \cup (\Sigma\backslash N^-)$. Since $w \notin N^+ \Delta N^- = (\Sigma\backslash N^+) \Delta (\Sigma\backslash N^-)$, we must have

$w \in (\Sigma\backslash N^+) \cap (\Sigma\backslash N^-)$. By the second part of our argument, since $E(w) \neq 0$, we have $w \in \Sigma_{\text{in}}$ and $w \in \Sigma_{\text{out}}$. This proves that $\Sigma'\backslash\Sigma_{\text{bound}} = \Sigma' \cap \Sigma_{\text{out}} = \Sigma' \cap \Sigma_{\text{in}}$. ∎

Now that we have asymptotic completeness we define the S-transformation.

Definition Let $\Sigma^{(\pm)} = (\Omega^{\pm})^{-1}[\Sigma'\backslash\Sigma_{\text{bound}}]$. The ***S*-transformation** is the map $S: \Sigma^{(+)} \to \Sigma^{(-)}$ defined by

$$Sw = (\Omega^-)^{-1}(\Omega^+ w)$$

Thus one has the picture shown schematically in Figure XI.1.

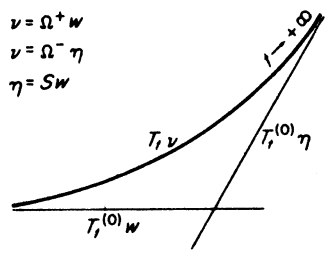


FIGURE XI.1 Schematic picture of scattering.

The S-transformation has thus been defined as a map from $\mathbb{R}^6$ to $\mathbb{R}^6$, or rather from $\mathbb{R}^6$ minus a set of measure 0 to $\mathbb{R}^6$. As a final topic in classical scattering theory, we shall describe a way of "reducing S" to two real-valued functions of two real variables in the case that $\mathbf{F}$ is a **central force**, that is, $V(\mathbf{r})$ is a function of $|\mathbf{r}| = r$ alone. First we note some symmetries of the S-operator. Since $\Omega^{\pm} T_t^{(0)} = T_t \Omega^{\pm}$, $ST_t^{(0)} = T_t^{(0)} S$. Since $E(\Omega^{\pm} w) = E_0(w)$, $E_0(Sw) = E_0(w)$. Finally, rotational invariance of F has two consequences. Let R be an element of $SO(3)$, the family of rotations on three-space. Define R on Σ by $R\langle r, v\rangle = \langle Rr, Rv\rangle$. Then $\Omega^{\pm}(Rw) = R(\Omega^{\pm} w)$, so $RS = SR$. Moreover, the angular momentum $\mathbf{L}\langle \mathbf{r}, \mathbf{v}\rangle = \mathbf{v} \times \mathbf{r}$ is conserved, so $\mathbf{L}(Sw) = \mathbf{L}(w)$. We summarize:

Proposition

(a) $ST_t^{(0)} = T_t^{(0)} S$.
(b) $SR = RS$.
(c) $E_0(S\,\cdot) = E_0(\cdot)$.
(d) $\mathbf{L}(S\,\cdot) = \mathbf{L}(\cdot)$.

Conditions (a) and (b) allow us to reduce S to a vector-valued function of only two variables. For the family of sets $\{RT_t^{(0)}w \mid t \in \mathbb{R}, R \in SO(3)\}$ foliates Σ into a two-parameter family of four-dimensional manifolds (with some exceptional manifolds of smaller dimension), the manifolds of constant E_0 and $|\mathbf{L}|$. By (a) and (b) if we know Sw for one w from each such manifold, we know S for all w. Because of (c) and (d), Sw can lie only on a two-dimensional manifold where E_0 and $\mathbf{L}$ are equal to their values at the point w. Thus we expect S to be parametrized by two real-valued functions of two real variables.

Let us be more explicit: By rotational invariance of S, it is enough to know $S(\mathbf{r}, \mathbf{v})$ when $\mathbf{v} = p\hat{z}$ and when $\mathbf{r}$ is in the y, z plane, where $\hat{z}$ is a unit vector in the z direction. If $S\langle \mathbf{r}, \mathbf{v}\rangle = \langle \mathbf{r}', \mathbf{v}'\rangle$, then by property (a), $S\langle \mathbf{r} + \mathbf{v}t, \mathbf{v}\rangle = \langle \mathbf{r}' + \mathbf{v}'t, \mathbf{v}'\rangle$, so we may suppose that $\mathbf{r} \cdot \mathbf{v} = 0$ or $\mathbf{r} = b\hat{y}$. To summarize, S may be recovered if we know $S\langle b\hat{y}, p\hat{z}\rangle$ for all real numbers b and p. Let $S\langle b\hat{y}, p\hat{z}\rangle = \langle \mathbf{r}', \mathbf{v}'\rangle$. By conservation of energy $|\mathbf{v}'| = p$ so $\mathbf{v}' = p\hat{\mathbf{e}}(b, p)$ where $\hat{\mathbf{e}}$ is some unit vector. By conservation of angular momentum, $\mathbf{r}'$ and $\mathbf{v}'$ lie in the y, z plane and the component of $\mathbf{r}'$ perpendicular to $\mathbf{v}'$ is determined. There are thus two functions that describe S: **the scattering angle** $\theta = \arccos(\hat{e} \cdot \hat{z})$ and the **time delay** $T = \mathbf{r}' \cdot \hat{e}/p$. These are written as functions of the momentum p and **impact parameter** b, or equivalently as functions of the energy $E = \frac{1}{2}p^2$ and angular momentum $\ell = pb$. One thus has the picture shown in Figure XI.2. Actually, one can explicitly solve the

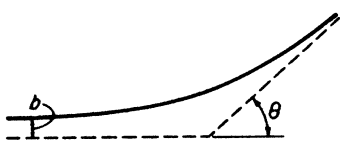


FIGURE XI.2 Central scattering.

central two-body problem up to quadratures and prove (see Problem 11 or the reference in the Notes):

$$\theta = \pi - 2\ell \int_{r_0(\ell, E)}^{\infty} [2E - 2V - r^{-2}\ell^2]^{-1/2} \frac{dr}{r^2} \tag{7a}$$

$$\begin{aligned} T = 2 &\int_{R_0}^{\infty} \{[2E - r^{-2}\ell^2]^{-1/2} - [2E - 2V - r^{-2}\ell^2]^{-1/2}\}\, dr \\ &-2 \int_{r_0(\ell, E)}^{R_0} [2E - 2V - r^{-2}\ell^2]^{-1/2}\, dr \\ &+2 \int_{\ell/\sqrt{2E}}^{R_0} [2E - r^{-2}\ell^2]^{-1/2}\, dr \end{aligned} \tag{7b}$$

where $r_0(\ell, E) = \sup\{r \mid V(r) + \ell^2/2r^2 > E\}$ and R_0 is any number larger than $\ell/\sqrt{2E}$ and r_0.

Notice that if $V = r^{-1}$ is substituted in (7a) and (7b), the integral for T diverges but the integral for θ converges. This remark will play an important role when we discuss Coulomb scattering in Section 9.

Finally, to make contact with physical experiments, we must define the cross section and its relation to the scattering angle θ. Let us return to the S-transformation in the general situation and consider a slightly different reduction from the one we discussed above. Write $S\langle \mathbf{r}, \mathbf{v}\rangle = \langle \mathbf{f}(\mathbf{r}, \mathbf{v}), \mathbf{g}(\mathbf{r}, \mathbf{v})\rangle$. We shall consider only $\mathbf{g}(\mathbf{r}, v\hat{z})$. We thus "throw away" the information in f which, in terms of our above analysis, is equivalent to ignoring the time delay. Suppose $v \neq 0$. The relation $ST_t^{(0)} = T_t^{(0)}S$ implies that $\mathbf{g}(\mathbf{r}, v\hat{z}) = \mathbf{g}(\mathbf{r} + \alpha\hat{z}, v\hat{z})$ for any $\alpha \in \mathbb{R}$; thus we consider only $\mathbf{g}(\mathbf{r}, v\hat{z})$ when $\mathbf{r} \cdot \hat{\mathbf{z}} = 0$. By conservation of energy $|\mathbf{g}| = v$, so $\hat{\mathbf{g}} = \mathbf{g}/v$. We have singled out the function $\hat{\mathbf{g}}(\mathbf{r}, v\hat{z})$. Fix v. $\hat{g}$ is then a map from $\mathbb{R}^2$, the plane orthogonal to $\hat{z}$ to the unit sphere S^2. Lebesgue measure on $\mathbb{R}^2$ then induces a measure σ on S^2 by

$$\sigma(E) = \mu(\hat{\mathbf{g}}^{-1}(E))$$

where μ is Lebesgue measure on $\mathbb{R}^2$ and E is a Borel subset of S^2. σ is called the **cross-section measure** on S^2. In most cases, σ is absolutely continuous with respect to the usual measure Ω on S^2 when the forward direction $\theta = 0$ is removed. Thus

$$d\sigma = \frac{d\sigma}{d\Omega}\, d\Omega$$

for a function $d\sigma/d\Omega$ on S^2 called the **differential cross section.**

Physical scattering experiments are well described by the following model: A beam of constant energy is sent toward the target. The beam has a wide spread and an approximately uniform density ρ of particles per unit area of the plane $\mathbb{R}^2$ orthogonal to the beam. A detector sits at some scattering angle $\langle \theta, \varphi\rangle$ far from the target and collects (and counts) all particles that leave the target within some angular region of size $\Delta\Omega$ about $\langle \theta, \varphi\rangle$. The measured quantity is

$$\frac{\text{number of particles hitting detector}}{(\Delta\Omega)\rho}$$

The reader should convince herself, that if $\Delta\Omega$ is very small, and the detector and source of particles are very far from the target, this quantity is very close to $d\sigma/d\Omega$. We also note that there is a formula for $(d\sigma/d\Omega)(\theta_0, \varphi_0)$ in the case where $F = -\nabla V$ with $V(r)$ a function of $|\mathbf{r}|$ alone, in terms of the

scattering angle θ as a function of E and b, the impact parameter. Explicitly (Problem 12),

$$\left.\frac{d\sigma}{d\Omega}\right|_{\theta=\theta_0} = \sum_{(b|\theta(b)=\theta_0)} b \csc\theta_0 \left(\frac{d\theta}{db}\right)^{-1} \tag{8}$$

in the case where the sum is finite.

XI.3 The basic principles of scattering in Hilbert space

Quantum dynamics is described by a unitary group on a Hilbert space. Also, as we have seen in Section X.13, the dynamics of classical wave equations can be naturally reformulated in terms of unitary groups. For this reason, the set of basic problems and principles that we present in this section are central to the variety of different scattering theories which we discuss in the remainder of the chapter. We begin with the definition of the generalized wave operators and describe the elementary "kinematics" associated to that notion. The existence of the wave operators is proven in most cases by a general technique known as Cook's method, which we present next. Under suitable conditions that are usually more stringent, one can prove existence *and* completeness by a complex of ideas associated with T. Kato and M. S. Birman. Cook's method and the Kato–Birman theory are the two pillars upon which the abstract time-dependent theory rests. In concrete cases one needs technical tools for showing that the hypotheses of these methods hold—some of these tools are discussed in Appendices 1 and 2 to this section. We end the section with a brief description of some of the ideas in the two Hilbert space theory and the corresponding Kato–Birman-type theorem.

Consider two unitary groups e^{-iAt} and e^{-iBt}, which we think of as an interacting dynamics and a comparison "free" dynamics. What does it mean for $e^{-iAt}\varphi$ to look "asymptotically free" as $t \to -\infty$? Clearly, it means that there is a vector φ_+ such that

$$\lim_{t\to-\infty} \|e^{-iBt}\varphi_+ - e^{-iAt}\varphi\| = 0 \tag{9}$$

Notice that (9) is equivalent to

$$\lim_{t\to-\infty} \|e^{iAt}e^{-iBt}\varphi_+ - \varphi\| = 0$$

so the basic existence question is reduced to the problem of proving the existence of strong limits. In most applications B has purely absolutely continuous spectrum; but in cases where it does not, we need to choose φ_+ in the absolutely continuous subspace for B. For example, if φ_+ were an eigenvector for B, then the strong limit above would exist only if φ_+ is also an eigenvector of A with the same eigenvalue (Problem 15). We therefore define the wave operators by first projecting onto the absolutely continuous subspace of B. When we discuss completeness, it will be clear that this is a very clever choice!

Definition Let A and B be self-adjoint operators on a Hilbert space $\mathscr{H}$ and let $P_{ac}(B)$ be the projection onto the absolutely continuous subspace of B. We say that the **generalized wave operators $\Omega^{\pm}(A, B)$ exist** if the strong limits

$$\Omega^{\pm}(A, B) = \operatorname*{s-lim}_{t\to\mp\infty} e^{iAt}e^{-iBt}P_{ac}(B) \tag{10}$$

exist. When $\Omega^{\pm}(A, B)$ exist, we define

$$\mathscr{H}_{in} = \operatorname{Ran}\Omega^{+} \qquad \text{and} \qquad \mathscr{H}_{out} = \operatorname{Ran}\Omega^{-}$$

For notational convenience, we sometimes use $\mathscr{H}_+$ for $\mathscr{H}_{in}$ and $\mathscr{H}_-$ for $\mathscr{H}_{out}$.

The strong limit in (10) turns out to be the right one to take. In case $P_{ac}(B) = 1$, the *norm* limit exists in (10) only if $A = B$ (Problem 15). On the other hand, as we shall see, if A has purely discrete spectrum, the weak limit in (10) exists (it is 0) even though A and B are very dissimilar.

The funny convention that $t \to \mp\infty$ corresponds to $\Omega^{\pm}$ is taken from the physics literature and is connected with the relation to the "time-independent theory": As we shall see in Section 6, Ω^{+} is related to $\lim_{\varepsilon\downarrow 0}(x + i\varepsilon - A)^{-1}$ and Ω^{-} to $\lim_{\varepsilon\downarrow 0}(x - i\varepsilon - A)^{-1}$.

The following proposition makes it clear that irrespective of its physical importance, scattering theory is a useful tool in spectral analysis—for this reason parts of this chapter and Chapter XIII are intimately related.

Proposition 1 Suppose that $\Omega^{\pm}(A, B)$ exist. Then:

(a) $\Omega^{\pm}$ are partial isometries with initial subspace $P_{ac}(B)\mathscr{H}$ and final subspaces $\mathscr{H}_{\pm}$.

(b) $\mathscr{H}_{\pm}$ are invariant subspaces for A and

$$\Omega^{\pm}[D(B)] \subset D(A), \qquad A\Omega^{\pm}(A, B) = \Omega^{\pm}(A, B)B \tag{11}$$

(c) $\mathscr{H}_{\pm} \subset \operatorname{Ran} P_{ac}(A)$.

Proof (a) If $u \in [P_{ac}(B)\mathscr{H}]^{\perp}$, then clearly $\Omega^{\pm}u = 0$. If $u \in P_{ac}(B)\mathscr{H}$, then $\|e^{iAt}e^{-iBt}P_{ac}(B)u\| = \|u\|$ for all t, so $\|\Omega^{\pm}(A, B)u\| = \|u\|$.

(b) Since

$$\text{s-lim}_{t \to \mp\infty} e^{iAt}e^{-iBt}P_{ac}(B) = \text{s-lim}_{t \to \mp\infty} e^{iA(t+s)}e^{-iB(t+s)}P_{ac}(B)$$

for any fixed s, we have that

$$\Omega^{\pm}(A, B) = e^{iAs}\Omega^{\pm}(A, B)e^{-iBs}$$

or equivalently,

$$e^{-iAs}\Omega^{\pm}(A, B) = \Omega^{\pm}(A, B)e^{-iBs} \tag{12}$$

(11) follows from Stone's theorem and (12). From (12) it is clear that $\mathscr{H}_{\pm}$ are invariant subspaces for e^{-iAs}.

(c) By (a) and (b), $A \restriction \mathscr{H}_{\pm}$ is unitarily equivalent to $B \restriction P_{ac}(B)\mathscr{H}$ where the unitary equivalence is given by $\Omega^{\pm} : P_{ac}(B)\mathscr{H} \to \mathscr{H}_{\pm}$. Thus $A \restriction \mathscr{H}_{\pm}$ is purely absolutely continuous. ∎

In quantum theory, where A and B are energy operators, (12) has an interpretation as energy conservation; see Section 4.

The following is often useful:

Proposition 2 (the chain rule) If $\Omega^{\pm}(A, B)$ and $\Omega^{\pm}(B, C)$ exist, then $\Omega^{\pm}(A, C)$ exist and

$$\Omega^{\pm}(A, C) = \Omega^{\pm}(A, B)\Omega^{\pm}(B, C)$$

Proof By Proposition 1c, Ran $\Omega^{\pm}(B, C) \subset$ Ran $P_{ac}(B)$, so

$$\lim_{t \to \mp\infty} \|(1 - P_{ac}(B))e^{itB}e^{-itC}P_{ac}(C)\varphi\| = 0$$

for any φ. Thus,

$$e^{itA}e^{-itC}P_{ac}(C)\varphi = e^{itA}e^{-itB}P_{ac}(B)e^{itB}e^{-itC}P_{ac}(C)\varphi + e^{itA}e^{-itB}(1 - P_{ac}(B))e^{itB}e^{-itC}P_{ac}(C)\varphi$$

converges to $\Omega^{\pm}(A, B)\,\Omega^{\pm}(B, C)\varphi$ as $t \to \mp\infty$ since a product of strongly convergent families of uniformly bounded operators is strongly convergent. ∎

As discussed in Section 1, weak asymptotic completeness says that $\mathscr{H}_{in} = \mathscr{H}_{out}$, while asymptotic completeness says $\mathscr{H}_{in} = \mathscr{H}_{out} = [P_{pp}(A)\mathscr{H}]^{\perp}$ where P_{pp} is the projection onto $\mathscr{H}_{pp}$, the span of the eigenvectors of A. For the abstract theory, a notion intermediate between these two is appropriate.

Definition Suppose that $\Omega^{\pm}(A, B)$ exist. We say that they are **complete** if and only if

$$\text{Ran } \Omega^{+} = \text{Ran } \Omega^{-} = \text{Ran } P_{ac}(A)$$

Thus asymptotic completeness is equivalent to the pair of statements: $\Omega^{\pm}$ are complete and $\sigma_{sing}(A) = \varnothing$. Since the latter statement is purely spectral, it is most naturally studied in a context partially disjoint from scattering theory. We discuss it in Chapter XIII.

The following remarkable fact reduces completeness to an existence question:

Proposition 3 Suppose that $\Omega^{\pm}(A, B)$ exist. Then they are complete if and only if $\Omega^{\pm}(B, A)$ exist.

Proof Suppose that both $\Omega^{\pm}(A, B)$ and $\Omega^{\pm}(B, A)$ exist. Then, by the chain rule, $P_{ac}(A) = \Omega^{\pm}(A, A) = \Omega^{\pm}(A, B)\Omega^{\pm}(B, A)$, so

$$P_{ac}(A)\mathscr{H} \subset \text{Ran } \Omega^{\pm}(A, B)$$

Since we already know that Ran $\Omega^{\pm}(A, B) \subset P_{ac}(A)\mathscr{H}$, completeness holds.

Conversely, suppose that $\Omega^{\pm}(A, B)$ exist and are complete. Let $\varphi \in P_{ac}(A)\mathscr{H}$. Then there is a ψ with $\varphi = \Omega^{\pm}(A, B)\psi$. By our discussion at the beginning of the section, this implies that

$$\|e^{-iAt}\varphi - e^{-iBt}P_{ac}(B)\psi\| \to 0$$

as $t \to -\infty$. Since e^{-iBt} is unitary,

$$\lim_{t \to -\infty} e^{iBt}e^{-iAt}\varphi$$

exists and equals $P_{ac}(B)\psi$. ∎

At first sight Proposition 3 seems to say that completeness is no harder than existence. In fact, usually completeness is much harder. The reason is that in applications B, which is the comparison free dynamics, is "simple," typically a constant coefficient partial differential operator (or pseudo-differential operator). With the resulting explicit formulas for e^{-iBt} one easily shows that $\Omega^{\pm}(A, B)$ exist by Cook's method. Since one does not have

explicit formulas for e^{-iAt}, it is not easy to show $\Omega^{\pm}(B, A)$ exist. Proposition 3 does suggest that one seek some condition on A and B which implies that $\Omega^{\pm}(A, B)$ exist and which is *symmetric* in A and B for then this condition will imply that both $\Omega^{\pm}(A, B)$ and $\Omega^{\pm}(B, A)$ exist, so $\Omega^{\pm}(A, B)$ will exist and be complete. This is the mechanism by which one obtains completeness in the Kato–Birman theory.

* * *

Cook's method is based on the observation that if f is a C^1 function on $\mathbb{R}$ with $f' \in L^1(\mathbb{R})$, then $\lim_{t\to\infty} f(t)$ exists since

$$|f(t) - f(s)| = \left| \int_s^t f'(u)\, du \right| \leq \int_s^t |f'(u)|\, du \to 0$$

as $s < t$ both go to ∞.

Theorem XI.4 (Cook's method) Let A and B be self-adjoint operators and suppose that there is a set $\mathscr{D} \subset D(B) \cap P_{ac}(B)\mathscr{H}$ which is dense in $P_{ac}(B)\mathscr{H}$ so that for any $\varphi \in \mathscr{D}$ there is a T_0 satisfying:

(a) For $|t| > T_0$, $e^{-iBt}\varphi \in D(A)$;

(b) $\int_{T_0}^{\infty} [\|(B - A)e^{-iBt}\varphi\| + \|(B - A)e^{+iBt}\varphi\|]\, dt < \infty$. (13)

Then $\Omega^{\pm}(A, B)$ exist.

Proof Let $\varphi \in \mathscr{D}$ and let $\eta(t) = e^{iAt}e^{-iBt}\varphi$. Since $e^{-itB}\varphi \in D(A) \cap D(B)$ for $t > T_0$, $\eta(t)$ is strongly differentiable on (T_0, ∞) and

$$\eta'(t) = -ie^{iAt}(B - A)e^{-iBt}\varphi$$

Thus for $t > s > T_0$,

$$\|\eta(t) - \eta(s)\| \leq \int_s^t \|\eta'(u)\|\, du \leq \int_s^t \|(B - A)e^{-iBu}\varphi\|\, du$$

goes to zero as $s \to \infty$ by (13). Thus $\eta(t)$ is Cauchy as $t \to \infty$, so $\lim_{t\to\infty} e^{iAt}e^{-iBt}P_{ac}(B)\psi$ exists for all $\psi \in \mathscr{D}$. The limit also exists trivially for all $\psi \in [P_{ac}(B)\mathscr{H}]^{\perp}$ and, so, by hypothesis for ψ lying in a dense set. Since the family $e^{iAt}e^{-iBt}P_{ac}(B)$ is a family of uniformly bounded operators, the existence of the limit for a dense set of ψ implies the existence of the limit for all ψ by an $\varepsilon/3$ argument. This proves that Ω^- exists. The proof for Ω^+ is identical. ∎

In applications, one needs to control $\|(B - A)e^{-iBt}\varphi\|$. When B is a constant coefficient differential operator, this can often be done by the method of stationary phase (see Appendix 1).

In some cases one wants a variety of extensions of this theorem. The following is useful when $B - A$ has various "local singularities"; see Section 4:

Theorem XI.5 (Kupsch–Sandhas theorem) Let A and B be self-adjoint operators and suppose that there is a bounded operator χ, and a subspace $\mathscr{D} \subset D(B) \cap P_{ac}(B)\mathscr{H}$ dense in $P_{ac}(B)\mathscr{H}$, so that for any $\varphi \in \mathscr{D}$, there is a T_0 satisfying:

(a) for $|t| > T_0$, $(1 - \chi)e^{-iBt}\varphi \in D(A)$;
(b) $\int_{T_0}^{\infty} [\|Ce^{-iBt}\varphi\| + \|Ce^{+iBt}\varphi\|]\, dt < \infty$;

where

$$C = A(1 - \chi) - (1 - \chi)B$$

Suppose, moreover, that for some n, $\chi(B + i)^{-n}$ is compact and that $\mathscr{D} \subset D(B^n)$. Then $\Omega^{\pm}(A, B)$ exist.

This result follows by a simple modification of the proof of Cook's method together with a general result which appears as Lemma 2 below. The reader is asked to provide a proof in Problem 19.

One problem with Cook's method is that it requires $B - A$ to be given to us as an operator rather than a quadratic form. The following result handles the form case:

Theorem XI.6 Let B be a positive self-adjoint operator and let $C_0, \ldots, C_n, D_0, \ldots, D_n$ be closed operators obeying:

(i) $D(C_i) \cap D(D_i) \supset Q(B)$ for $i = 1, \ldots, n$, and

$$\|C_i\varphi\|^2 \leq \alpha_i(\varphi, B\varphi) + \beta_i\|\varphi\|^2, \qquad \|D_i\varphi\|^2 \leq \alpha_i(\varphi, B\varphi) + \beta_i\|\varphi\|^2$$

for all $\varphi \in Q(B)$.

(ii) $C_0 = 1$, $Q(D_0) \supset Q(B)$, and

$$|(\varphi, D_0\varphi)| \leq \alpha_0(\varphi, B\varphi) + \beta_0(\varphi, \varphi)$$

for all $\varphi \in Q(B)$.

(iii) The quadratic form $\sum_{i=0}^{n} C_i^* D_i$ defined on $Q(B)$ is symmetric and $\sum_{i=0}^{n} \alpha_i < 1$.

(iv) There is a set $\mathscr{D}$ contained in Ran $P_{ac}(B) \cap D(B)$ which is dense in $P_{ac}(B)\mathscr{H}$, so that for $\varphi \in \mathscr{D}$,

$$\int_{-\infty}^{\infty} \sum_{i=0}^{n} \|D_i e^{-iBt}\varphi\|\, dt < \infty$$

Then the form sum $A = B + \sum_{i=0}^{n} C_i^* D_i$ is a self-adjoint operator and $\Omega^{\pm}(A, B)$ exist.

Proof By (i), (ii), and (iii), $\sum_{i=0}^{n} C_i^* D_i$ is a relatively form bounded perturbation of B with relative bound $\alpha \equiv \sum_{i=0}^{n} \alpha_i < 1$. It follows that A is self-adjoint and that $Q(A) = Q(B)$. In particular, the norms

$$\|\varphi\|_B = \|(B+1)^{1/2}\varphi\|, \qquad \|\varphi\|_A = \|(A+E)^{1/2}\varphi\|$$

on $Q(B)$ are equivalent norms, that is,

$$c_1\|\varphi\|_B \leq \|\varphi\|_A \leq c_2\|\varphi\|_B$$

Here E is some fixed number so that $A + E \geq 1$. e^{-iBt} is clearly an isometry in $\|\cdot\|_B$. Since e^{-iAt} is an isometry in $\|\cdot\|_A$, by the above equivalence, we have that

$$\|e^{-iAt}\varphi\|_B \leq c\|\varphi\|_B \tag{14}$$

with $c = c_1^{-1}c_2$ independent of t. Let $W(t) = e^{iAt}e^{-iBt}$. Then for $\varphi \in \mathscr{D}$ and $t \geq s$,

$$\|(W(t) - W(s))\varphi\|^2 = (W(t)\varphi, (W(t) - W(s))\varphi) - (W(s)\varphi, (W(t) - W(s))\varphi)$$

We shall prove that as $t, s \to \infty$, each of these terms goes to zero, so that, as in Cook's theorem, $\Omega^{\pm}(A, B)$ exist. We consider the first term; the second is similar. We first claim that

$$(W(t)\varphi, (W(t) - W(s))\varphi) = i\int_s^t \sum_{j=0}^{n} (C_j e^{-iAu}W(t)\varphi, D_j e^{-iBu}\varphi)\, du \tag{15}$$

(15) follows (Problem 20) from the hypotheses and the fact that by (14) e^{-iAu} and e^{-iBu} take $Q(B)$ into itself. By (14) and the hypotheses (i), (ii), for all t, u,

$$\sup_j \|C_j e^{-iAu}W(t)\varphi\| \leq \gamma\|\varphi\|_B$$

for some γ (*independent of* t *and* u). It follows by (15) that

$$|(W(t)\varphi, (W(t) - W(s))\varphi)| \leq \gamma\|\varphi\|_B \int_s^t \sum_{j=0}^{n} \|D_j e^{-iBu}\varphi\|\, du$$

As in Cook's theorem, by hypothesis (iv), this goes to zero as $s, t \to \infty$. ∎

* * *

We now turn to the complex of results that we designate as the Kato–Birman theory. This theory uses the notion of trace class operator developed in Section VI.6. To describe the idea behind the theory, suppose that $B - A$ is a rank one operator, that is, $(B - A)\varphi = (\psi, \varphi)\psi$. If we tried to use Cook's method to show that $\Omega^{\pm}(A, B)$ exist, we would seek φ with $(\psi, e^{-iBt}\varphi) \in L^1(\mathbb{R})$. Since $\varphi \in P_{ac}(B)\mathscr{H}$, we know that the spectral measure $d(\varphi, E_\lambda\varphi)$ equals $|f(\lambda)|^2\, d\lambda$ for some f. We shall see below that it follows that $d(\psi, E_\lambda\varphi) = g(\lambda)|f(\lambda)|^2\, d\lambda$ for some g in $L^2(\mathbb{R}, f^2\, d\lambda)$, and thus

$$(\psi, e^{-iBt}\varphi) = \int e^{-it\lambda}g(\lambda)|f(\lambda)|^2\, d\lambda$$

Therefore, $(\psi, e^{-iBt}\varphi)$ is the Fourier transform of $(2\pi)^{1/2}g|f|^2$. In general, it is not easy to see when a Fourier transform is in L^1 but to get it to be in L^2 is easy. We therefore begin by finding a set of φ with $(\psi, e^{-iBt}\varphi) \in L^2(\mathbb{R})$.

Definition Let B be a self-adjoint operator and $\{E_\Omega\}$ its spectral family. $\mathscr{M}(B)$ will denote the set of all $\varphi \in \mathscr{H}$ such that $d(\varphi, E_\lambda\varphi) = |f(\lambda)|^2\, d\lambda$ where $f \in L^\infty(\mathbb{R})$. We let $|||\varphi|||$ be the L^∞-norm of f.

It is not hard (Problem 17) to prove that $|||\cdot|||$ is a norm and that $\mathscr{M}(B)$ is dense (in the $\mathscr{H}$-norm) in Ran $P_{ac}(B)$.

Lemma 1 For any $\varphi \in \mathscr{M}(B)$ and any $\psi \in \mathscr{H}$,

$$\int |(\psi, e^{-iBt}\varphi)|^2\, dt \leq 2\pi\|\psi\|^2|||\varphi|||^2 \tag{16}$$

Proof Let Q be the projection onto the cyclic subspace generated by B and φ. Let $d(\varphi, E_\lambda\varphi) = |f(\lambda)|^2\, d\lambda$. By general spectral theory (see Chapter VII and Section VIII.3) $Q\mathscr{H}$ is unitarily equivalent to $L^2(\mathbb{R}, |f(\lambda)|^2\, d\lambda)$ in such a way that φ corresponds to the vector $\varphi(\lambda) \equiv 1$ and e^{-iBt} is multiplication by $e^{-it\lambda}$. Let $\eta(\lambda)$ correspond to the vector $Q\psi$. Then

$$(\psi, e^{-iBt}\varphi) = (Q\psi, e^{-iBt}\varphi) = \int \eta(\lambda)|f(\lambda)|^2 e^{-it\lambda}\, d\lambda \tag{17}$$

so, by the Plancherel theorem,

$$\int |(\psi, e^{-iBt}\varphi)|^2\, dt = 2\pi \int |\eta(\lambda)|^2|f(\lambda)|^4\, d\lambda$$

$$\leq 2\pi\|f\|_\infty^2 \int |\eta(\lambda)|^2|f(\lambda)|^2\, d\lambda$$

By definition $\|f\|_\infty = |||\varphi|||$ and

$$\int |\eta(\lambda)|^2|f(\lambda)|^2\, d\lambda = \|Q\psi\|^2 \leq \|\psi\|^2 \quad ∎$$

We shall need another simple consequence of thinking of the unitary group in terms of the Fourier transform:

Lemma 2 For any $\varphi \in P_{ac}(B)$, $e^{-itB}\varphi \to 0$ weakly as $t \to \pm\infty$. If C is compact, then $\|Ce^{-itB}\varphi\| \to 0$ as $t \to \pm\infty$.

Proof By (17) and the fact that f and ηf are in L^2, we have that $(\psi, e^{-itB}\varphi)$ is the Fourier transform of an L^1 function. So, by the Riemann–Lebesgue lemma (Theorem IX.7), $(\psi, e^{-itB}\varphi) \to 0$. Thus, $\|Fe^{-itB}\varphi\| \to 0$ for any finite rank operator F. The result for compact operators follows by an $\varepsilon/3$ argument. ∎

We shall derive the results in the Kato–Birman theory from the following theorem.

Theorem XI.7 (Pearson's theorem) Let A and B be self-adjoint operators and let J be a bounded operator. Suppose that there is a trace class operator C so that $C = AJ - JB$ in the sense that for all $\varphi \in D(A)$ and $\psi \in D(B)$,

$$(\varphi, C\psi) = (A\varphi, J\psi) - (\varphi, JB\psi)$$

then

$$\Omega^{\pm}(A, B; J) \equiv \operatorname*{s-lim}_{t \to \mp\infty} e^{iAt}Je^{-iBt}P_{ac}(B)$$

exist.

Proof Let $W(t) = e^{iAt}Je^{-iBt}$ and consider the case $t \to \infty$. By the density argument of Cook's method, it suffices to show that

$$\lim_{t<s;\, t\to\infty} \|(W(t) - W(s))\varphi\|^2 = 0 \tag{18}$$

for all $\varphi \in \mathscr{M}(B)$. We shall prove this by writing the left-hand side as two pieces, one to be controlled by Lemma 1 and one by Lemma 2. Let

$$F_{ab}(X) = \int_a^b e^{iBt}Xe^{-iBt}\,dt$$

for a bounded operator X and $a < b$. We first claim that

$$W(t)^*W(s) - e^{iaB}W(t)^*W(s)e^{-iaB} = F_{0a}(Y(t, s)) \tag{19}$$

where

$$Y(t, s) = -i[e^{itB}J^*e^{-i(t-s)A}Ce^{-isB} - e^{itB}C^*e^{-i(t-s)A}Je^{-isB}]$$

We shall prove (19) without worrying about domain questions, leaving the reader to take matrix elements and fill in these domain details. The idea will be to write the difference on the left as the integral of its derivative. Let

$$Q(b) = e^{ibB}W(t)^*W(s)e^{-ibB}$$

Then

$$\begin{aligned}\frac{dQ(b)}{db} &= ie^{ibB}[Be^{itB}J^*e^{-i(t-s)A}Je^{-isB} - e^{itB}J^*e^{-i(t-s)A}Je^{-isB}B]e^{-ibB} \\ &= ie^{ibB}[e^{itB}J^*e^{-i(t-s)A}Ce^{-isB} - e^{itB}C^*e^{-i(t-s)A}Je^{-isB}]e^{-ibB} \\ &= -e^{ibB}Y(t, s)e^{-ibB}\end{aligned}$$

Thus (19) follows by integrating the derivative.

For fixed t and s,

$$W(t) - W(s) = i\int_s^t e^{iuA}Ce^{-iuB}\,du$$

is compact, so by Lemma 2,

$$\lim_{a\to\infty} e^{iaB}W(t)^*(W(t) - W(s))e^{-iaB}\varphi = 0$$

for $\varphi \in \mathscr{M}(B)$. It follows by (19) that for $\varphi \in \mathscr{M}(B)$,

$$(\varphi, W(t)^*(W(t) - W(s))\varphi) = \lim_{a\to\infty} (\varphi, F_{0a}(Y(t, t) - Y(t, s))\varphi) \tag{20}$$

Since C is trace class, it has an expansion (see (VI.6)):

$$C = \sum_{n=1}^{\infty} \lambda_n(\varphi_n, \cdot)\psi_n$$

where $\sum \lambda_n = \|C\|_1$, the trace class norm of C, and with $\{\varphi_n\}$ and $\{\psi_n\}$ orthonormal and $\lambda_n > 0$. We claim that for any bounded operator X and $a > 0$,

$$\begin{aligned}&|(\varphi, F_{0a}(e^{iuB}XCe^{-iuB})\varphi)| \\ &\quad \le (2\pi\|C\|_1)^{1/2}\|X\|\,|||\varphi|||\left[\sum_n \lambda_n \int_u^{\infty} |(\varphi_n, e^{-ixB}\varphi)|^2\,dx\right]^{1/2}\end{aligned} \tag{21}$$

For, by the canonical expansion above,

$$\begin{aligned}\text{LHS of (21)} &\le \left| \sum_n \lambda_n \int_u^{a+u} (e^{-ixB}\varphi, X\psi_n)(\varphi_n, e^{-ixB}\varphi)\, dx \right| \\ &\le \left[\sum_n \lambda_n \int_{-\infty}^{\infty} |(X\psi_n, e^{-ixB}\varphi)|^2\, dx \right]^{1/2} \\ &\quad \times \left[\sum_n \lambda_n \int_u^{\infty} |(\varphi_n, e^{-ixB}\varphi)|^2\, dx \right]^{1/2} \\ &\le \text{RHS of (21)}\end{aligned}$$

In the second line we used the Schwarz inequality (twice). In the last step, we used Lemma 1. By (20) and (21)

$$\begin{aligned}\|(W(t) - W(s))\varphi\|^2 &\le 8(2\pi\|C\|_1)^{1/2}|||\varphi||| \, \|J\| \\ &\quad \times \left[\sum_n \lambda_n \int_{\min(t,s)}^{\infty} |(\varphi_n, e^{-ixB}\varphi)|^2\, dx \right]^{1/2} \qquad (22)\end{aligned}$$

In the first place, this equation and Lemma 1 imply that

$$\|(W(t) - W(s))\varphi\|^2 \le 16\pi\|C\|_1 |||\varphi|||^2 \|J\| \qquad (23)$$

and, in the second place, since $\sum_n \lambda_n |(\varphi_n, e^{-ixB}\varphi)|^2$ is in L^1, (18) follows. ∎

As a corollary of the theorem and (23), we have:

Corollary Under the hypotheses of Theorem XI.7,

$$\|[\Omega^{\pm}(A, B; J) - J]\varphi\|^2 \le 16\pi\|C\|_1 |||\varphi|||^2 \|J\| \qquad (24)$$

Proof In (23) take $s = 0$ and let $t \to \pm\infty$. ∎

If $AJ - JB$ is trace class, then so is $BJ^* - J^*A$, so both s-lim $e^{iAt}Je^{-iBt}P_{ac}(B)$ and s-lim $e^{iBt}J^*e^{-iAt}P_{ac}(A)$ exist. For general J, this does not imply completeness of either strong limit (for example, consider $J = 0$); but if $J = 1$, Proposition 3 is applicable, so we immediately have the corollary:

Theorem XI.8 (Kato–Rosenblum theorem) If A and B are self-adjoint operators with $A - B \in \mathscr{I}_1$, the trace class, then $\Omega^{\pm}(A, B)$ exist and are complete.

In this theorem A and B may be unbounded. $A - B$ trace class is intended in the sense of Theorem XI.7, that is, $(A\varphi, \psi) = (\varphi, B\psi) + (\varphi, C\psi)$ for some $C \in \mathscr{I}_1$ and $\varphi \in D(A)$, $\psi \in D(B)$. It then follows that $D(A) = D(B)$ and $A\varphi = B\varphi + C\varphi$ for $\varphi \in D(A)$.

Corollary Let $\{A_n\}_{n=1}^{\infty}$, A, B be self-adjoint operators. Suppose that $\Omega^{\pm}(A, B)$ exist and that each $A_n - A$ is trace class with $\|A_n - A\|_1 \to 0$ as $n \to \infty$. Then, for each n, $\Omega^{\pm}(A_n, B)$ exist and

$$\Omega^{\pm}(A, B) = \text{s-lim } \Omega^{\pm}(A_n, B)$$

as $n \to \infty$. If $\Omega^{\pm}(B, A)$ exist, then for each n, $\Omega^{\pm}(B, A_n)$ exist and

$$\Omega^{\pm}(B, A)\varphi = \lim_{n\to\infty} \Omega^{\pm}(B, A_n)\varphi$$

for all $\varphi \in \text{Ran } P_{ac}(A)$.

Proof By the chain rule, it suffices to prove that

$$\text{s-lim}_{n\to\infty} \Omega^{\pm}(A_n, A) = P_{ac}(A) \qquad (25)$$

and

$$\lim_{n\to\infty} \Omega^{\pm}(A, A_n)\varphi = \varphi \qquad \text{for} \quad \varphi \in \text{Ran } P_{ac}(A) \qquad (26)$$

From the corollary to Theorem XI.7 we immediately conclude that (25) holds. Let φ be in Ran $P_{ac}(A)$ and let $\varphi_n = \Omega^{+}(A_n, A)\varphi$. By (25), $\|\varphi_n - \varphi\| \to 0$ as $n \to \infty$. Thus,

$$\|\Omega^{+}(A, A_n)(\varphi_n - \varphi)\| \to 0$$

But, by the completeness of $\Omega^{+}(A_n, A)$, we have that $\Omega^{+}(A, A_n)\varphi_n = \varphi$, so the last limit result says that (26) holds. ∎

It can happen that for $\varphi \in [\text{Ran } P_{ac}(A)]^{\perp}$, $\Omega^{\pm}(B, A_n)\varphi$ does not go to zero as $n \to \infty$ (Problem 22).

One cannot replace the trace class condition in Theorem XI.8 by a condition that $A - B$ be Hilbert–Schmidt or that $A - B$ be any $\mathscr{I}_p$ with $p > 1$; see the discussion in the Notes. One problem with Theorem XI.8 is that in quantum mechanics $B - A$ is not even bounded.

Theorem XI.9 (Kuroda–Birman theorem) Let A and B be self-adjoint operators so that $(A + i)^{-1} - (B + i)^{-1} \in \mathscr{I}_1$. Then $\Omega^{\pm}(A, B)$ exist and are complete.

Proof Let $J = (A + i)^{-1}(B + i)^{-1}$. Then, in the sense of expectation values,

$$AJ - JB = (B + i)^{-1} - (A + i)^{-1}$$

is trace class, so by Pearson's theorem

$$\text{s-lim}_{t \to \pm\infty} e^{iAt}(A + i)^{-1}(B + i)^{-1}e^{-iBt}P_{ac}(B)$$

exist. Applying this to a vector of the form $(B + i)\varphi$ with $\varphi \in D(B)$, we conclude that

$$\text{s-lim}_{t \to \pm\infty} e^{iAt}(A + i)^{-1}e^{-iBt}P_{ac}(B)$$

exist. Now, by hypothesis, $(A + i)^{-1} - (B + i)^{-1}$ is compact, so by Lemma 2,

$$\text{s-lim}_{t \to \pm\infty}[(A + i)^{-1} - (B + i)^{-1}]e^{-iBt}P_{ac}(B) = 0$$

It follows that

$$\text{s-lim}_{t \to \pm\infty} e^{iAt}(B + i)^{-1}e^{-iBt}P_{ac}(B)$$

exist. Applying this to a vector of the form $(B + i)\varphi$, we conclude that $\Omega^{\pm}(A, B)$ exist. It follows by symmetry that $\Omega^{\pm}(B, A)$ exist and thus completeness holds. ∎

To state the next result, we need a technical definition:

Definition Let A and B be self-adjoint operators. We say that A is **subordinate** to B if there are continuous functions f and g on $\mathbb{R}$ with $f(x) \geq 1$, $g(x) \geq 1$, and $\lim_{|x| \to \infty} f(x) = \infty$ such that $D(g(B)) \subset D(f(A))$ and $f(A)g(B)^{-1}$ is bounded. If A is subordinate to B and B is subordinate to A, we say they are **mutually subordinate**.

This condition is very weak. For example, by the closed graph theorem, if $D(A) = D(B)$ or if A and B are semibounded and $Q(A) = Q(B)$, they are mutually subordinate.

Theorem XI.10 (Birman's theorem) Suppose that A and B are self-adjoint operators with spectral projections $E_{\Omega}(A)$, $E_{\Omega}(B)$, respectively. Assume that:

(a) $E_I(A)(A - B)E_I(B) \in \mathscr{I}_1$ for every bounded interval I.
(b) A and B are mutually subordinate.

Then $\Omega^{\pm}(A, B)$ exist and are complete.

Proof By symmetry and Proposition 3, it suffices to show that $\Omega^{\pm}(A, B)$ exist. Let $E_a(C) \equiv E_{(-a,a)}(C)$ and $E'_a(C) = E_{(-\infty,-a]\cup[a,\infty)}(C)$ where C is A or B. If $J = E_a(A)E_a(B)$, then $AJ - JB \in \mathscr{I}_1$ by hypothesis (a), so

$$\text{s-lim}_{t \to \pm\infty} e^{iAt}E_a(A)E_a(B)e^{-iBt}$$

exist by Pearson's theorem. Let $\varphi \in \text{Ran } E_{a_0}(B)$ for some a_0. Then for $a > a_0$ we have that

$$\lim_{t \to \pm\infty} e^{iAt}E_a(A)e^{-iBt}\varphi$$

exist, so to conclude that $\Omega^{\pm}(A, B)\varphi$ exist, it suffices to show that

$$\lim_{a \to \infty} \left[\sup_t \|E'_a(A)e^{-iBt}\varphi\|\right] = 0 \tag{27}$$

Now, let f and g be the functions given by the condition that A is subordinate to B. Let $F(a) = \inf_{|x| \geq a} f(x)$. Then $F(a) \to \infty$ as $a \to \infty$ since $f \to \infty$. Thus:

$$\begin{aligned}\|E'_a(A)e^{-iBt}\varphi\| &\leq F(a)^{-1}\|f(A)E'_a(A)e^{-iBt}\varphi\| \\ &\leq F(a)^{-1}\|f(A)g(B)^{-1}\|\,\|g(B)e^{-iBt}\varphi\| \\ &\leq F(a)^{-1}\|f(A)g(B)^{-1}\|\left[\sup_{|x| \leq a_0}|g(x)|\right]\|\varphi\|\end{aligned}$$

so that (27) holds. ∎

The Kuroda–Birman and Birman theorems have corollaries involving strong convergence similar to the previous corollaries. We leave those to the problems (Problems 23, 24).

There are a large number of conditions that arise in applications but which are not covered by the above considerations. For example, suppose that $A \geq 0$, $B \geq 0$ and $A^2 - B^2 \in \mathscr{I}_1$. Do $\Omega^{\pm}(A, B)$ exist? Or consider $A = -\Delta + V$; $B = -\Delta$ on $\mathbb{R}^n$. For $n \geq 4$, $(A + i)^{-1} - (B + i)^{-1}$ is not trace class for any nontrivial V; but, as we shall see, $(A + E)^{-k} - (B + E)^{-k}$ is trace class so long as k is large enough. Does this imply that $\Omega^{\pm}(A, B)$ exist? The answer to both questions is yes because of the general principle which we are about to describe.

Definition A function φ on T, an open subset of $\mathbb{R}$, is called **admissible** if $T = \bigcup_1^N I_n$ where $I_n = (\alpha_n, \beta_n)$ are disjoint, N is finite or infinite, and:

(a) The distributional derivative φ'' is L^1 on each compact subinterval of T;
(b) on each interval (α_n, β_n), φ' is either *strictly* positive or *strictly* negative.

Example 1 If $T = (0, \infty) = I_1$, then $\varphi(x) = x^{1/2}$ is admissible. Notice that if $A^2 = A_1$, $B^2 = B_1$, then, so long as $A, B \geq 0$, $A = \varphi(A_1)$, $B = \varphi(B_1)$, and $A_1 - B_1 \in \mathscr{I}_1$ if $A^2 - B^2 \in \mathscr{I}_1$.

Example 2 If $T = (0, \infty) = I_1$, then $\varphi(x) = x^{-1/n} - a$ is admissible. Notice that if $A > -a$, $B > -a$, and $A_1 = (A + a)^{-n}$, $B_1 = (B + a)^{-n}$, then $A = \varphi(A_1)$, $B = \varphi(B_1)$, and $A_1 - B_1 \in \mathscr{I}_1$ if $(A + a)^{-n} - (B + a)^{-n} \in \mathscr{I}_1$.

Theorem XI.11 (invariance principle—trace class case) Let φ be an admissible function on an open set T. Suppose that A and B are self-adjoint operators with $\sigma(A), \sigma(B) \subset \bar{T}$ and that at each boundary point of T either φ has a finite limit or both A and B do not have point spectrum at that point. Suppose that $A - B$ is trace class. Then $\Omega^{\pm}(\varphi(A), \varphi(B))$ exist, are complete, and

$$\Omega^{\pm}(\varphi(A), \varphi(B)) = \Omega^{\pm}(A, B)E_{T_1}(B) + \Omega^{\mp}(A, B)E_{T_2}(B)$$

where T_1 (respectively, T_2) is the union of those intervals where $\varphi' > 0$ (respectively, $\varphi' < 0$).

More generally, the same conclusion holds if the condition $A - B \in \mathscr{I}_1$ is replaced by either the hypotheses of Birman's theorem or of the Kuroda–Birman theorem.

The condition at the boundary points is put in only so that $\varphi(A)$ and $\varphi(B)$ can be properly defined.

Before proving this theorem we note that there is a version of it in the case where Cook's method is applicable; see Appendix 3. We also note that on account of Examples 1 and 2 and a continuation of the two examples we have:

Corollary 1 If A and B are positive operators with $A^2 - B^2 \in \mathscr{I}_1$, then $\Omega^{\pm}(A, B)$ exist and are complete.

Corollary 2 If A and B are positive operators with $(A^2 + 1)^{-1} - (B^2 + 1)^{-1} \in \mathscr{I}_1$, then $\Omega^{\pm}(A, B)$ exist and are complete.

Corollary 3 If A and B are operators with $A, B \geq -a + I$ and $(A + a)^{-k} - (B + a)^{-k} \in \mathscr{I}_1$ for some k, then $\Omega^{\pm}(A, B)$ exist and are complete.

Corollary 4 If A and B are self-adjoint operators and $e^{-A} - e^{-B} \in \mathscr{I}_1$, then $\Omega^{\pm}(A, B)$ exist and are complete.

We return below to conditions which guarantee that the hypotheses of Corollary 3 hold. A weak version of Corollary 3 which is sufficient for all applications can be also proven by the method we used to prove Theorem XI.9 (Problem 25). As preparation for the proof of Theorem XI.11, we need:

Lemma 3 Let φ be an admissible function. Then:

(a) If $Y \subset \mathbb{R}$ has Lebesgue measure zero, then $\varphi[Y \cap T]$ and $\varphi^{-1}[Y]$ have measure zero.

(b) For any $w \in L^2(\alpha_n, \beta_n)$ with $\varphi' > 0$ on (α_n, β_n),

$$\lim_{s \to \infty} \int_0^\infty \left| \int_{-\infty}^{\infty} e^{-i(t\lambda + s\varphi(\lambda))} w(\lambda)\, d\lambda \right|^2 dt = 0 \tag{28}$$

If $\varphi' < 0$ on (α_n, β_n), $s \to \infty$ should be replaced by $s \to -\infty$ in (28).

Proof (a) See Problem 26.

(b) Since $(2\pi)^{-1/2} \int_{-\infty}^{\infty} e^{i(t\lambda + s\varphi(\lambda))} w(\lambda)\, d\lambda$ is the inverse Fourier transform of $e^{is\varphi(\lambda)} w(\lambda)$, the Plancherel theorem implies that

$$2\pi \|w\|^2 \geq \int_0^\infty \left| \int_{-\infty}^{\infty} e^{i(t\lambda + s\varphi(\lambda))} w(\lambda)\, d\lambda \right|^2 dt$$

Thus we need prove (28) only for a set of w whose linear combinations are dense in $L^2(\alpha_n, \beta_n)$, say for w the characteristic function of $[a, b] \subset (\alpha_n, \beta_n)$. Since φ'' is L^1 on (α_n, β_n), φ is a C^1 function and thus $\inf_{\lambda \in [a, b]} \varphi'(t) = \gamma > 0$. Using

$$e^{-i(t\lambda + s\varphi(\lambda))} = i(t + s\varphi'(\lambda))^{-1} \frac{d}{d\lambda} (e^{-i(t\lambda + s\varphi(\lambda))})$$

for $t > 0$, $s > 0$, we see that

$$\begin{aligned} &\left| \int_a^b e^{-i(t\lambda + s\varphi(\lambda))}\, d\lambda \right| \\ &\quad = \left| \int_a^b (t + s\varphi'(\lambda))^{-1} \frac{d}{d\lambda} e^{-i(t\lambda + s\varphi(\lambda))}\, d\lambda \right| \\ &\quad \leq (t + s\varphi'(b))^{-1} + (t + s\varphi'(a))^{-1} + (t + s\gamma)^{-2} s \int_a^b |\varphi''(\lambda)|\, d\lambda \end{aligned}$$

where we integrate by parts to get to the last inequality. Taking $s \to \infty$ and noting that each term goes to zero in $L^2(0, \infty)$ as a function of t, (28) results. ∎

Proof of Theorem XI.11 Let $C \equiv A - B = \sum \lambda_n(\psi_n, \cdot)\psi_n$ and let

$$\eta \in \text{Ran } E_{(\alpha_n, \beta_n)}(B) \cap \mathscr{M}(B).$$

Then, by (22),

$$\|(\Omega^{\pm}(A, B) - 1)e^{-i\varphi(B)s}\eta\|^2 \leq c\left(\sum_{n=1}^{\infty} |\lambda_n| \int_0^{\infty} |(\psi_n, e^{-iBt - i\varphi(B)s}\eta)|^2 \, dt\right)^{1/2} \tag{29}$$

Now, by Lemma 3b, the individual integrals on the right-hand side of (29) go to zero as $s \to \infty$ (respectively, $s \to -\infty$) if $\varphi' > 0$ ($\varphi' < 0$). Since each integral is bounded on account of Lemma 1 by $2\pi\|\psi_n\|^2\|\eta\|\|^2$ and $\sum |\lambda_n| \|\psi_n\|^2 = \text{Tr}(|C|) < \infty$, the sum on the right-hand side of (29) goes to zero. By Proposition 1, $\Omega^{\pm}(A, B)e^{-i\varphi(B)s} = e^{-i\varphi(A)s}\Omega^{\pm}(A, B)$, so

$$\lim_{s \to \pm\infty} e^{i\varphi(A)s}e^{-i\varphi(B)s}\eta = \begin{cases} \Omega^{\mp}(A, B)\eta & (\varphi' > 0) \\ \Omega^{\pm}(A, B)\eta & (\varphi' < 0) \end{cases}$$

By Lemma 3a, $P_{\text{ac}}(\varphi(B)) = P_{\text{ac}}(B)$, so the theorem is proven in the case where $A - B$ is trace class.

To prove the theorem under the more general hypotheses, one proceeds as follows: If $AJ - JB$ is in $\mathscr{I}_1$, then

$$\text{s-lim}_{t \to \pm\infty} e^{i\varphi(A)t}Je^{-i\varphi(B)t}$$

exist and obey a formula analogous to the invariance principle. The proof is identical to the one above. By using this more general result and employing the J's used in the proofs of the Kuroda–Birman and Birman theorems, the invariance principle can be extended to these cases also. The J's are functions of A and B rather than $\varphi(A)$ and $\varphi(B)$. Again, we leave the continuity result to the reader (Problem 28). ∎

Theorem XI.12 Let B be a positive self-adjoint operator and suppose that C is a symmetric form bounded perturbation of B with relative bound $\alpha < 1$ and that

$$(B + 1)^{-\frac{1}{4}}C(B + 1)^{-k-\frac{1}{4}} \in \mathscr{I}_1 \tag{30}$$

Then $A = B + C$ is the form of a self-adjoint operator obeying

$$(A + E)^{-k} - (B + E)^{-k} \in \mathscr{I}_1 \tag{31}$$

for all sufficiently large E. In particular, $\Omega^{\pm}(A, B)$ exist and are complete.

Proof The last statement follows from (31) and the third corollary of Theorem XI.11. By repeated use of

$$(A + E)^{-1} = (B + E)^{-1} - (A + E)^{-1}C(B + E)^{-1}$$

we find that

$$(A + E)^{-k} = (B + E)^{-k} - \sum_{j=1}^{k} (A + E)^{-j}C(B + E)^{-k+j-1}$$

so that (31) follows from

$$(A + E)^{-j}C(B + E)^{-k-1+j} \in \mathscr{I}_1, \qquad j = 1, \ldots, k \tag{32}$$

By a complex interpolation argument (Problem 29a), this follows from

$$(A + E)^{-\frac{1}{4}}C(B + E)^{-k-\frac{1}{4}} \in \mathscr{I}_1, \qquad (A + E)^{-k-\frac{1}{4}}C(B + E)^{-\frac{1}{4}} \in \mathscr{I}_1 \tag{33}$$

The first part of (33) follows from the hypothesis (30) and the fact that $(A + E)^{-\frac{1}{4}}(B + 1)^{\frac{1}{4}}$ is bounded. We need only prove the second part of (33) for E very negative. Choose E so negative that

$$\|(B + E)^{-\frac{1}{4}}C(B + E)^{-\frac{1}{4}}\| = \gamma < 1 \tag{34}$$

Then,

$$(A + E)^{-1} = (B + E)^{-\frac{1}{4}}\left\{\sum_{j=0}^{\infty} [-(B + E)^{-\frac{1}{4}}C(B + E)^{-\frac{1}{4}}]^j\right\}(B + E)^{-\frac{1}{4}}$$

so that

$$(B + E)^{-\frac{1}{4}}(A + E)^{-k}C(B + E)^{-\frac{1}{4}} = \sum (-1)^{m-1}\left[\prod_{i=1}^{m} (B + E)^{-\frac{1}{4}-\ell_i}C(B + E)^{-\frac{1}{4}}\right] \tag{35}$$

with the sum over a suitable family of terms with $\ell_1 + \cdots + \ell_m = k$. By a complex interpolation between (30) and (34) (Problem 29b),

$$(B + E)^{-\frac{1}{4}-\ell_i}C(B + E)^{-\frac{1}{4}} \in \mathscr{I}_{k/\ell_i}, \qquad \ell_i = 1, \ldots, k \tag{36}$$

where $\mathscr{I}_p$ is the trace ideal of the appendix to Section IX.4. Using Hölder's inequality for these trace ideals on each term in (35), employing (34) for factors with $\ell_i = 0$ and (36) for terms with $\ell_i > 0$, we see that each term on the right of (35) is in $\mathscr{I}_1$ with a norm bounded by const γ^m. The γ^m makes the sum converge in (35) so that $(B + E)^{-\frac{1}{4}}(A + E)^{-k}C(B + E)^{-\frac{1}{4}}$ is in $\mathscr{I}_1$. Since $(A + E)^{-\frac{1}{4}}(B + E)^{+\frac{1}{4}}$ is bounded, the second part of (33) holds. ∎

The point is that (30) can be verified in a number of applications when B is a differential operator and C is a lower order operator. The main abstract result is described in Appendix 2.

* * *

We close this section with a few words about two Hilbert space scattering theory. In Section 10, we describe physical systems in which the two Hilbert space theory is natural. In that section we give a method for reducing the two Hilbert space problem to a problem on a single space. In typical applications, one can use either that reduction theory or Theorem XI.13 below.

Definition Let B and A be self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively, and let J be a bounded operator from $\mathscr{H}_1$ to $\mathscr{H}_2$. We say that $\Omega^{\pm}(A, B; J)$ exist if and only if the strong limits

$$\Omega^{\pm}(A, B; J) = \operatorname*{s-lim}_{t \to \mp\infty} e^{iAt} J e^{-iBt} P_{ac}(B)$$

exist.

$\Omega^{\pm}(A, B; J)$ may not be isometries. Nevertheless:

Proposition 4 $(\operatorname{Ker} \Omega^{+})^{\perp} \equiv \mathscr{H}'_{in}$ is an invariant space for B and $\mathscr{H}_{in} = \overline{\operatorname{Ran} \Omega^{+}}$ is an invariant space for A. Further, $B \restriction \mathscr{H}'_{in}$ is *unitarily* equivalent to $A \restriction \mathscr{H}_{in}$. In particular, $A \restriction \mathscr{H}_{in}$ is purely absolutely continuous.

Proof As in the usual theory,

$$e^{-iAt}\Omega^{+} = \Omega^{+} e^{-iBt} \tag{37}$$

from which it follows that e^{-iBt} (respectively, e^{-iAt}) leaves $\mathscr{H}'_{in}$ (respectively, $\mathscr{H}_{in}$) invariant. The polar decomposition of an operator from $\mathscr{H}_1$ to itself is easily seen to extend to operators from $\mathscr{H}_1$ to $\mathscr{H}_2$. The result is that Ω^{+} has a decomposition $\Omega^{+} = V|\Omega^{+}|$ with $|\Omega^{+}| = [(\Omega^{+})^{*}\Omega^{+}]^{1/2}$ in $\mathscr{L}(\mathscr{H}_1)$ and V a partial isometry with initial space $\mathscr{H}'_{in}$ in $\mathscr{H}_1$ and final subspace $\mathscr{H}_{in} \subset \mathscr{H}_2$. We claim that

$$e^{-iAt}V = Ve^{-iBt} \tag{38}$$

from which the claimed unitary equivalence will follow. By (37), $(\Omega^{+})^{*}e^{-iAt} = e^{-iBt}(\Omega^{+})^{*}$, whence

$$(\Omega^{+})^{*}\Omega^{+}e^{-iBt} = (\Omega^{+})^{*}e^{-iAt}\Omega^{+} = e^{-iBt}(\Omega^{+})^{*}(\Omega^{+})$$

By the uniqueness of the positive square root (Theorem VI.9),

$$|\Omega^{+}|e^{-iBt} = e^{-iBt}|\Omega^{+}|$$

so (37) implies that

$$e^{-iAt}V|\Omega^{+}| = Ve^{-iBt}|\Omega^{+}|$$

As a result, (38) holds applied to vectors in $\overline{\operatorname{Ran} |\Omega^{+}|}$. To complete the proof of (38), we note that for vectors φ in $(\operatorname{Ran} |\Omega^{+}|)^{\perp} = \operatorname{Ker} |\Omega^{+}| = \operatorname{Ker} V$, one clearly has that $e^{-iAt}V\varphi = 0$. Moreover, $Ve^{-iBt}\varphi = 0$ since we have seen that e^{-iBt} leaves $\operatorname{Ker} |\Omega^{+}| = (\mathscr{H}'_{in})^{\perp}$ invariant. ∎

It is easy to see that the chain rule now says that if $\Omega^{\pm}(A, B; J_1)$ and $\Omega^{\pm}(B, C; J_2)$ exist, then so do $\Omega^{\pm}(A, C; J_1 J_2)$ and they equal $\Omega^{\pm}(A, B; J_1)\Omega^{\pm}(B, C; J_2)$.

One phenomenon that can occur is that $\mathscr{H}'_{in}$ may not be $\operatorname{Ran} P_{ac}(B)$; for example, take $J = 0$.

Definition If $(\operatorname{Ker} \Omega^{\pm})^{\perp} = \operatorname{Ran} P_{ac}(B)$, we call $\Omega^{\pm}$ **semicomplete**. If also $\overline{\operatorname{Ran} \Omega^{\pm}} = \operatorname{Ran} P_{ac}(A)$, we call $\Omega^{\pm}$ **complete**.

In physical situations it can often happen that there is some arbitrariness in the choice of J. It is therefore important to have criteria which guarantee that $\Omega^{\pm}(A, B; J_1) = \Omega^{\pm}(A, B; J_2)$.

Definition We say that two operators $J_1, J_2 \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ are **asymptotically *B*-equivalent** if

$$\operatorname*{s-lim}_{t \to \pm\infty} \{(J_1 - J_2)e^{-iBt} P_{ac}(B)\} = 0$$

In most applications one proves this by showing that $J_1 - J_2$ is compact or that $(J_1 - J_2)(B + i)^{-k}$ is compact for some k (Problem 18).

Definition Let $J \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ and $J' \in \mathscr{L}(\mathscr{H}_2, \mathscr{H}_1)$. We say that J' is a ***B*-asymptotic left inverse for *J*** (*B*-left inverse for short) if and only if $J'J$ is asymptotically B-equivalent to I.

The following analogue to Proposition 3 is left to the reader (Problem 30):

Proposition 5 Let B and A be self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively. Let $J \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ and suppose that $\Omega^{\pm}(A, B; J)$ exist.

(a) Let $J_1 \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$. Then J_1 is asymptotically B-equivalent to J if and only if $\Omega^{\pm}(A, B; J_1)$ exist *and* equal $\Omega^{\pm}(A, B; J)$.
(b) If J has a B-left inverse, then $\Omega^{\pm}$ are semicomplete.
(c) Let J' be any B-left inverse. Then $\Omega^{\pm}(A, B; J)$ are complete if and only if $\Omega^{\pm}(B, A; J')$ exist *and* J is an A-asymptotic left inverse for J'.
(d) If J^* is a B-left inverse for J, then $\Omega^{\pm}(A, B; J)$ are partial isometries with initial space Ran $P_{ac}(B)$.

We note that Pearson's theorem holds without any change in statement *and* proof if one defines $\mathscr{I}_1(\mathscr{H}_1, \mathscr{H}_2)$ as those operators $A \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ with $(A^*A)^{1/2} \in \mathscr{I}_1(\mathscr{H}_1)$.

Theorem XI.13 (Belopol'skii–Birman theorem) Let B and A be self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively, with spectral resolutions $E_\Omega(A)$ and $E_\Omega(B)$. Suppose that $J \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ satisfies:

(a) J has a two-sided bounded inverse.
(b) For any bounded interval I,

$$E_I(A)(AJ - JB)E_I(B) \in \mathscr{I}_1$$

(c) For any bounded interval I, $(J^*J - 1)E_I(B)$ is compact;

and *either*:

(d_1) $JD(B) = D(A)$;

or

(d_2) $JQ(B) = Q(A)$.

Then $\Omega^{\pm}(A, B; J)$ exist, are complete, and are partial isometries with initial space Ran $P_{ac}(B)$ and final space Ran $P_{ac}(A)$.

Proof Let $J_I = E_I(A)JE_I(B)$ and $J_I' = E_I(B)J^{-1}E_I(A)$. By the generalized Pearson result and (b), the operators $\Omega^{\pm}(A, B; J_I)$ and $\Omega^{\pm}(B, A; J_I^*)$ exist. Moreover, we claim that J_I' is asymptotically A-equivalent to J_I^*. For, by (c), $E_I(B)(J^*J - 1)$ is compact, so $E_I(B)(J^* - J^{-1})$ is compact and thus $J_I^* - J_I'$ is compact. By Lemma 2 we have the claimed asymptotic equivalence. Thus $\Omega^{\pm}(B, A; J_I')$ exist by (a) of Proposition 5.

By hypothesis (d), we can use the method of Theorem XI.10 to show that

$$\lim_{a \to \infty} \left| \sup_t (\| E_{(-\infty, -a) \cup (a, \infty)}(A) J e^{-iBt} \varphi \|) \right| = 0$$

for $\varphi \in$ Ran $E_I(B)$, so $\Omega^{\pm}(A, B; J)$ exist. Similarly, $\Omega^{\pm}(B, A; J^{-1})$ exist. It follows by (c) of Proposition 5 that $\Omega^{\pm}(A, B; J)$ is complete. Using hypothesis (c) *again*, we conclude from (d) of Proposition 5 and Lemma 2 that $\Omega^{\pm}(A, B; J)$ are partial isometries from Ran $P_{ac}(B)$ to Ran $P_{ac}(A)$. ∎

Appendix 1 to XI.3: Stationary phase methods

In this appendix we present a method for estimating $[e^{-itB}]\varphi(x)$ in the case where B is a differential or pseudo-differential operator. We then illustrate how the estimates can be used by showing that $\Omega^{\pm}(A, B)$ exist when $A - B$ is multiplication by a suitable function. Finally, we discuss how the estimates can be used to handle the second-order wave equations of Sections 10 and 16.

The key to this method is the idea of stationary phase. We shall rewrite $e^{-itB}\varphi(x)$ as $\int u(k)e^{i\omega f(k)}\,dk$ where $\omega \to \infty$ as $t \to \infty$. As $\omega \to \infty$, the rapid oscillations in $e^{i\omega f(k)}$ tend to cancel one another. The cancellation is least effective at points where f varies most slowly, that is, points with $(\nabla f)(k) = 0$. These are called points of **stationary phase**. We first control the integral at points with $\nabla f \neq 0$ and then analyze the points of stationary phase.

Given an open set $\mathcal{O} \subset \mathbb{R}^n$, let $C^\ell(\mathcal{O})$ denote the ℓ-times differentiable functions on $\mathcal{O}$ topologized as a Fréchet space by using the seminorms

$$\|f\|_K = \sup_{k \in K} \sum_{|\alpha| \leq \ell} |D^\alpha f(k)|$$

K running through all compact subsets of $\mathcal{O}$. We first prove a result that singles out the points of stationary phase in the asymptotics of integrals of the form $\int e^{i\omega f(k)}u(k)\,dk$.

Theorem XI.14 Let K be a compact subset of $\mathbb{R}^n$. Suppose that f is a real-valued function defined on a neighborhood $\mathcal{O}$ of K such that $f \in C^{\ell+1}(\mathcal{O})$ with grad f nonvanishing on all of K. Then, for all $u \in C_0^\ell(K^{\text{int}})$,

$$\left| \int e^{i\omega f(k)}u(k)\,dk \right| \leq c(1 + |\omega|)^{-\ell}\|u\|_{\ell,\infty} \tag{39}$$

where

$$\|u\|_{\ell,\infty} = \sum_{|\alpha| \leq \ell} \|D^\alpha u\|_\infty$$

Moreover, if $M \subset C^{\ell+1}(\mathcal{O})$ is a compact subset of $C^{\ell+1}$ with $(\text{grad } f)(k)$ nonvanishing for all $k \in K$ and $f \in M$, then the constant c in (39) can be chosen uniformly for all $f \in M$.

Proof First fix f. For each $k \in K$, we can find a neighborhood U_k of k, $a_k > 0$, and $j \in \{1, \dots, n\}$ so that $|\partial f/\partial k_j| \geq a_k$ for all points in U_k. By the compactness of K, we can cover it with finitely many such sets $U_1, \dots, U_n$. Now find $\varphi_1, \dots, \varphi_n \in C_0^\infty(\mathcal{O})$ so that $\text{supp } \varphi_i \subset U_i$ and $\sum \varphi_i(y) = 1$ if $y \in K$. By writing

$$e^{i\omega f(k)}u(k) = \sum_j e^{i\omega f(k)}(u\varphi_j)(k)$$

and using $\|\varphi_j u\|_{\ell,\infty} \leq C\|u\|_{\ell,\infty}$, we see that we are reduced to considering the case where $\partial f/\partial k_1 \geq a > 0$ on all of K.

Since $\partial f/\partial k_1 \neq 0$ on K, we can find, by the implicit function theorem, a neighborhood V_k of any $k \in K$ and a $C^{\ell+1}$ function g so that $g(f(k), k_2, \dots, k_n) = \langle k_1, \dots, k_n\rangle$ for all $k \in V_k$. By using the partition of unity $\{\varphi_i\}$ as above, we can suppose that one g works on all of K. Let $\langle y_1, \dots, y_n\rangle = \langle f(k), k_2, \dots, k_n\rangle$. Then

$$\begin{aligned}\int u(k)e^{i\omega f(k)}\,dk &= \int u(g(y))e^{i\omega y_1}\left[\frac{\partial f}{\partial k_1}(g(y))\right]^{-1} dy \\ &= \int \left[\left(\frac{1}{i\omega}\frac{\partial}{\partial y_1}\right)^{\ell} e^{i\omega y_1}\right](u \circ g)\left(\frac{\partial f}{\partial k_1}\right)^{-1} dy \\ &= \omega^{-\ell}\int e^{i\omega y_1}\left(i\frac{\partial}{\partial y_1}\right)^{\ell}\left[(u \circ g)\left(\frac{\partial f}{\partial k_1}\right)^{-1}\right] dy\end{aligned}$$

Thus,

$$(1 + |\omega|)^{\ell}\left|\int u(k)e^{i\omega f(k)}\,dk\right| \leq D\|(u \circ g)(\partial f/\partial k_1)^{-1}\|_{\ell,\infty}$$

proving (39).

Looking at the above proof, we see that for some neighborhood N of f in $C^{\ell+1}(\mathcal{O})$, we can use the same U_k, etc., and so obtain (39) with a fixed constant c' for all $f \in N$. Covering M with such neighborhoods, we obtain the final uniformity statement. ∎

Corollary Let $P: \mathbb{R}^n \to \mathbb{R}$ be C^∞ and let $u \in \mathcal{S}(\mathbb{R}^n)$ be a function so that $\hat{u}$ has compact support. Let $\mathcal{G}$ be an open set containing the compact set $\{\text{grad } P(k) \mid k \in \text{supp } \hat{u}\}$. Let

$$u_t(\mathbf{x}) = (2\pi)^{-n/2}\int \exp[i(\mathbf{x}\cdot\mathbf{k} - tP(\mathbf{k}))]\hat{u}(\mathbf{k})\,d\mathbf{k} \tag{40a}$$

Then, for any m, there is a c depending on m, u, and $\mathcal{G}$ so that

$$|u_t(\mathbf{x})| \leq c(1 + |\mathbf{x}| + |t|)^{-m} \tag{40b}$$

for all $\mathbf{x}$, t with $\mathbf{x}/t$ not in $\mathcal{G}$.

Proof Let $f(k) = (|\mathbf{x}| + |t|)^{-1}[x \cdot k - tP(k)]$ and $\omega = |\mathbf{x}| + |t|$ so that (40) has the form of (39). Since $\nabla_k f = (|\mathbf{x}| + |t|)^{-1}[x - t\,\nabla_k P]$, if $x/t \notin \mathcal{G}$, then $\nabla_k f$ is nonvanishing. Moreover, we can take $x/t \to \infty$ in a fixed direction and get limiting functions whose gradients do not vanish either. Thus, the f's lie in a suitable compact subset of C^{m+1} which yields (40b). ∎

(40) has a beautiful and simple interpretation. Think of a classical system with momentum k and Hamiltonian function $P(k)$ independent of x. Such a system has a constant velocity $v = \nabla P(k)$. Thus a classical "packet" $\hat{u}(k)$ has velocities v in $\mathcal{G}$. (40) says that outside of this classically allowed region, the "quantum" wave packet $u_t(x)$ falls off very rapidly. Next we investigate the contribution of isolated points where grad f vanishes:

Theorem XI.15 Let f be a C^∞ real-valued function defined in a neighborhood of 0 in $\mathbb{R}^n$. Suppose that $(\text{grad } f)(0) = 0$ and that the matrix $A_{ij} = (\partial^2 f/\partial k_i\,\partial k_j)(0)$ is invertible. Then there is a neighborhood $\mathcal{O}$ of 0 such that for any $s > n/2$ there is a c so that for all $u \in C_0^\infty(\mathcal{O})$ and $\omega \geq 1$,

$$\left|\int u(k)e^{i\omega f(k)}\,dk\right| \leq c\omega^{-n/2}\|u\|_{s,\infty} \tag{41}$$

Moreover, given such an f_0, there exist neighborhoods $\mathcal{O}_1$ and $\mathcal{O}_2$ of zero with $\bar{\mathcal{O}}_1 \subset \mathcal{O}_2 \subset \mathcal{O}$, and a neighborhood $\mathcal{N}$ of f_0 in the $C^\ell(\mathcal{O}_2)$ topology (for some ℓ) so that (41) holds for all $u \in C_0^\infty(\mathcal{O}_1)$ and $f \in \mathcal{N}$.

Proof First fix an f satisfying the hypotheses of the theorem. We claim that there exists an $\mathcal{O}$ and a C^∞ invertible map $X: \mathcal{O} \to \mathcal{O}'$ such that $X(k) = k + O(k^2)$ and such that

$$f(k) = f(0) + \tfrac{1}{2}(X(k), AX(k)) \tag{42}$$

Since $(\text{grad } f)(0) = 0$, by Taylor's theorem with remainder, we have

$$f(k) = f(0) + \tfrac{1}{2}(B(k)k, k)$$

where

$$(B(k))_{ij} = 2\int_0^1 \frac{\partial^2 f}{\partial k_i\,\partial k_j}(sk)(1 - s)\,ds$$

We now seek a C^∞ $n \times n$ matrix-valued function $R(k)$ so that

$$R^*(k)AR(k) = B(k)$$

for if we then take $X(k) = R(k)k$, (42) will hold. Let M be the vector space of $n \times n$ matrices and M_s be the vector space of symmetric $n \times n$ matrices. Consider the function F from $M \times M_s$ to M_s given by

$$F(R, B) = R^*AR - B$$

Thus $(D_R F)|_{R=I,\, B=A}$, the gradient in the R variables, is the map T from M to M_s given by

$$T(C) = C^*A + AC$$

Given $D \in M_s$, $T(\frac{1}{2}A^{-1}D) = D$; so T is surjective since A is nonsingular. Since $F(I, A) = 0$, it follows by the implicit function theorem that for some neighborhood $\mathscr{A}$ of A, there is a C^∞ function $R\colon \mathscr{A} \to M$ so that

$$R^*(B)AR(B) = B, \qquad R(A) = 1$$

Pick $\mathcal{O}$ so that $B(k) \in \mathscr{A}$ for $k \in \mathcal{O}$. Let

$$X(k) = R(B(k))k$$

Then X is C^∞, obeys (42), and, since $B(k) = A + O(k)$, $R(B(k)) = 1 + O(k)$ so that $X(k) = k + O(k^2)$.

Now, letting $y = X(k)$,

$$\left|\int u(k)e^{i\omega f(k)}\,dk\right| = \left|\int u(X^{-1}(y))e^{i\omega\langle y,\, Ay\rangle/2}\left[\det\left(\frac{\partial X}{\partial k}\circ X^{-1}(y)\right)\right]^{-1} dy\right|$$

$$= \left|\int v(y)e^{i\omega\langle y,\, Ay\rangle/2}\,dy\right|$$

with $v(y) = u(X^{-1}(y))[\det(\partial X/\partial k \circ X^{-1}(y))]^{-1}$. By the Plancherel theorem,

$$\int v(y)e^{i\omega\langle y,\, Ay\rangle/2}\,dy = c_1\omega^{-n/2}\int \check{v}(k)e^{-i\langle k,\, A^{-1}k\rangle/2\omega}\,dk \tag{43}$$

for a suitable A-dependent constant c_1. Thus

$$\left|\int u(k)e^{i\omega f(k)}\,dk\right| \le |c_1|\omega^{-n/2}\|\check{v}\|_1$$

$$\le c_2\omega^{-n/2}\|(1-\Delta)^{n/2}v\|_2$$

$$\le c\omega^{-n/2}\|u\|_{s,\,\infty}$$

It remains to prove the uniformity statement at the end of the theorem.

We first claim that for all f near f_0 in the $C^2(\mathcal{O})$ topology, there exists a unique point $k(f)$ near zero with

$$(\text{grad } f)(k(f)) = 0$$

To see this, let $\mathscr{G}\colon \mathcal{O} \times C^2(\mathcal{O}) \to \mathbb{R}^n$ be the map

$$\mathscr{G}(k, f) = (\text{grad } f)(k)$$

Then $\mathscr{G}(0, f_0) = 0$ and $D_k\mathscr{G}|_{k=0,\, f=f_0}$ is the invertible map A. The claim thus follows from the implicit function theorem. We can therefore conclude that the uniformity statement holds by noting that the size of $\mathcal{O}$ and the constant c in the above proof depend only on finitely many derivatives. ∎

Corollary Let P be a C^∞ function on $\mathbb{R}^n$ and let $u \in \mathscr{S}(\mathbb{R}^n)$ be a function such that $\hat{u}$ has compact support and such that

$$\text{supp } \hat{u} \cap \{k \,|\, \det[\partial^2 P/\partial k_i\, \partial k_j] = 0\}$$

is empty. Let $u_t(x)$ be given by (40a). Then

$$|u_t(x)| \le c|t|^{-n/2} \tag{44}$$

for $|t| > 1$ and all x.

Proof Let $\mathscr{J}$ be a bounded neighborhood of supp $\hat{u}$ such that $\det[\partial^2 P/\partial k_i\, \partial k_j] \neq 0$ for $k \in \overline{\mathscr{J}}$. By the corollary to Theorem XI.14, we need only verify (44) for x/t in $\mathscr{G} = \{\text{grad } P(k) \,|\, k \in \mathscr{J}\}$. For each $p = x/t$ in $\mathscr{G}$,

$$\nabla_k[(|x| + |t|)^{-1}(x \cdot k - tP(k))]$$

vanishes at a finite number of points in $\mathscr{J}$ so that using a partition of unity and Theorem XI.15, (44) holds for $p = x/t$. By the uniformity part of that theorem, the estimate actually holds for a neighborhood of p. By the compactness of $\overline{\mathscr{G}}$, (44) holds for all x and t. ∎

To see how these estimates can be used in scattering theory, consider:

Theorem XI.16 Let P be a C^∞ real-valued function on $\mathbb{R}^n$ such that

$$M \equiv \{k \,|\, \text{grad } P(k) = 0 \text{ or } \det(\partial^2 P/\partial k_i\, \partial k_j) = 0\}$$

has measure zero. Let V be a real-valued function on $\mathbb{R}^n$ such that

$$(1 + |x|)^{-m}V \in L^2 \tag{45a}$$

We can take $\rho = \frac{1}{2}(1 + \max \rho_\pm)$. (a) is essentially a kind of finite propagation speed for the Klein–Gordon equation. Since the initial data do not have compact support in x, we cannot expect the solution to vanish when $|x|$ is large compared to t, but it does decay rapidly. Notice that for this kind of "finite propagation speed," the speed is actually less than one.

For use in Section 16, we note the following corollary to Theorem XI.17.

Corollary If φ is a regular wave packet for the Klein–Gordon equation (46) with $m \neq 0$, then

$$\int_{\mathbb{R}^n} |\varphi(x, t)|\, dx \leq C(1 + |t|)^{n/2}$$

Proof Break up the x integral into two pieces: $|x| \leq t$ and $|x| \geq t$. By (b), the first integral is bounded by

$$d(1 + |t|)^{-n/2} \int_{|x| \leq t} d^n x \leq c_1 |t|^{n/2}$$

By (a), the second integral goes to zero faster than any power of $|t|$ and in particular is bounded by c_2. Take $C = \max\{c_1, c_2\}$. ∎

Now consider the case $m = 0$. Theorem XI.14 is applicable and immediately yields

$$|\varphi(x, t)| \leq c_{M,\varepsilon}(|x| + |t| + 1)^{-M} \quad \text{if} \quad |x| \geq (1 + \varepsilon)|t| \quad \text{or} \quad |x| \leq (1 - \varepsilon)|t|$$

We emphasize the requirement that $0 \notin \operatorname{supp} u_\pm$ when $m = 0$, for the last estimate will be false in dimension $n = 1$ if $g = \widehat{\varphi_t(\cdot, 0)}$ satisfies $g(0) \neq 0$. In fact, in one dimension, solutions of $\varphi_{tt} = \varphi_{xx}$ with initial data in $\mathscr{S}$ obey

$$\lim_{t \to \infty} \varphi(x, t) = \frac{1}{2} \int_{-\infty}^{\infty} \varphi_t(y, 0)\, dy \tag{47}$$

for any *fixed* x, so that $\varphi(x, t)$ does not go to zero for $|x| \leq (1 - \varepsilon)|t|$. (47) follows from the explicit form of the solution in one dimension:

$$\varphi(x, t) = \frac{1}{2} \int_{x-t}^{x+t} \varphi_t(y, 0)\, dy + \frac{1}{2}[\varphi(x + t, 0) + \varphi(x - t, 0)]$$

This formula also shows that in the case $n = 1$, $\|\varphi\|_\infty$ does not fall off as $|t|^{-n/2}$; in fact the proof of falloff when $m > 0$ fails to extend since $\{M_{ij}\}$ is no longer invertible. However, $\{M_{ij}\}$ is nonsingular in $n - 1$ directions; so we

expect, and shall prove, that φ obeys

$$|\varphi(x, t)| \leq d|t|^{-(n-1)/2} \tag{48}$$

It is sufficient to prove (48) in any fixed x direction as long as d is independent of x, so we take $x = \langle x_1, 0, \ldots, 0\rangle$, $x_1 > 0$. Thus, we need to control

$$\varphi_\pm(x, t) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{\pm it|k| + ik_1 x_1} u_\pm(k)\, d^n k$$

We shall control φ_- for t positive; the other proofs are similar. Choose $\varepsilon > 0$ so that u_- vanishes in the ball of radius 2ε about zero. Pick χ_1 and χ_2 in $C^\infty(\mathbb{R}^n)$ so that $\chi_1 + \chi_2 = 1$ and $\chi_1(k) = 0$ if $k_1 < \varepsilon$ and $\chi_2(k) = 0$ if $k_1 > \frac{3}{2}\varepsilon$. Write

$$\varphi_-(x, t) = (2\pi)^{-n/2} \int_{k_1 > \varepsilon} e^{-it|k| + ik_1 x_1} \chi_1(k) u_-(k)\, dk + (2\pi)^{-n/2} \int_{\substack{k_1 < 3\varepsilon/2 \\ |k| \geq 2\varepsilon}} e^{-it|k| + ik_1 x_1} \chi_2(k) u_-(k)\, dk$$

Since $\nabla_k(-t|k| + k_1 x_1)$ vanishes only when $k_1 > 0$, $k_2 = \cdots = k_n = 0$, the second region of integration contains no points of stationary phase, and so the second integral vanishes faster than any power of t. Thus, we need control only the first integral. We do this by introducing a change of variables which separates the direction of the line of stationary phase. Define

$$K_1(k) = k_1$$

$$K_j(k) = \frac{k_j}{\sqrt{k_2^2 + \cdots + k_n^2}} (|k| - k_1)^{1/2}, \qquad j = 2, \ldots, n$$

Then $k \to K$ is a diffeomorphism on $\mathscr{N} = \{k | k_1 > \varepsilon\}$. Since

$$|k| = K_1 + \sum_{j=2}^{n} K_j(k)^2$$

we have, for suitable g and h,

$$\left| (2\pi)^{-n/2} \int_{\mathscr{N}} e^{-it|k| + ik_1 x_1} \chi_1(k) u_-(k)\, d^n k \right|$$

$$= \left| (2\pi)^{-n/2} \int_{K[\mathscr{N}]} \exp\left[iK_1(x_1 - t) - it \sum_{j=2}^{n} K_j^2 \right] g(K)\, d^n K \right|$$

$$\leq t^{-(n-1)/2} \int_{\mathbb{R}^{n-1}} \left| \exp\left(-(4ti)^{-1} \sum_{j=2}^{n} y_j^2 \right) \right| |h(x_1 - t, y_2, \ldots, y_n)|\, d^{n-1} y$$

from which the estimate (48) follows. We summarize:

Theorem XI.18 Let φ be a regular wave packet for the wave equation (46) with $m = 0$. Then:

(a) For any $\varepsilon > 0$ and any N, there is a $c_{N,\varepsilon}$ so that

$$|\varphi(x, t)| \leq c_{N,\varepsilon}(1 + |x| + |t|)^{-N}$$

if $|x| < (1 - \varepsilon)|t|$ or $|x| > (1 + \varepsilon)|t|$.

(b) For some d,

$$|\varphi(x, t)| \leq d|t|^{-(n-1)/2}$$

for all x and t.

Our definition of regular wave packet when $m = 0$ includes the condition that the Fourier transforms of the initial data vanish near the origin. Actually, this hypothesis is not necessary for part (b). In fact, using either explicit formulas for the solution or further stationary phase analysis (Problem 33), one can prove that the following holds:

Theorem XI.19 Let $\varphi(x, t)$ be a solution of (46) in the case $m = 0$ with initial data in $\mathscr{S}(\mathbb{R}^n)$. Then:

(a) For any N and $\varepsilon > 0$, there is a $c_{N,\varepsilon}$ so that

$$|\varphi(x, t)| \leq c_{N,\varepsilon}(1 + |x| + |t|)^{-N}, \qquad |x| \geq (1 + \varepsilon)|t|$$

(b) For any $\varepsilon > 0$, there is a c so that

$$|\varphi(x, t)| \leq c_{\varepsilon}(1 + |t|)^{-(n-1)}, \qquad |x| \leq (1 - \varepsilon)|t|$$

(c) There is a d so that

$$|\varphi(x, t)| \leq d(1 + |t|)^{-(n-1)/2} \qquad \text{all } x \text{ and } t$$

When n is even, the result in (b) is the best possible. In fact, if $h = \varphi(\cdot, 0) = 0$ and $\ell = \varphi_t(\cdot, 0)$ is in C_0^∞, then, for x fixed, $\varphi(x, t) \sim c_n t^{-(n-1)} \int \ell(y)\, dy$ with $c_n \neq 0$ if n is even. But when n is odd and greater than one. Huygens' principle assures us that the estimate of part (a) also holds in the region $|x| \leq (1 - \varepsilon)|t|$ of part (b).

Appendix 2 to XI.3: Trace ideal properties of $f(x)g(-i\nabla)$

To apply the theorems of the Kato–Birman theory, it is often necessary to prove that certain operators of the form $f(x)g(-i\nabla)$ are trace class. Such operators arise in a variety of other situations also, and it is sometimes sufficient to know weaker information about the singular values $\{\mu_m\}$ than $\sum |\mu_m| < \infty$. Recall that $\mathscr{I}_p$ is the set of A in $\mathscr{L}(\mathscr{H})$ such that $\|A\|_p \equiv (\mathrm{tr}(|A|^p))^{1/p} < \infty$. Properties of $\mathscr{I}_p$ and $\|\cdot\|_p$ may be found in Section VI.6 and in the appendix to Section IX.4. The following results are true:

Theorem XI.20 Let $2 \leq q < \infty$ and suppose that $f, g \in L^q(\mathbb{R}^n)$. Then $f(x)g(-i\nabla)$ is in $\mathscr{I}_q$ and

$$\|f(x)g(-i\nabla)\|_q \leq (2\pi)^{-n/q}\|f\|_q\|g\|_q$$

Recall that $L^2_\delta(\mathbb{R}^n)$ is the set of f such that $\|f\|_\delta = \|(1 + x^2)^{\delta/2}f(x)\|_{L_2} < \infty$.

Theorem XI.21 Suppose that f and g are in $L^2_\delta(\mathbb{R}^n)$ for some $\delta > n/2$. Then $f(x)g(-i\nabla)$ is a trace class operator and

$$\|f(x)g(-i\nabla)\|_1 \leq c_{\delta,n}\|f\|_\delta\|g\|_\delta$$

There exist necessary and sufficient conditions that $f(x)g(-i\nabla)$ be trace class (see the Notes). In applications, Theorem XI.21 suffices.

Theorem XI.22 Let $2 < q < \infty$ and suppose that $g \in L^q_w(\mathbb{R}^n), f \in L^q(\mathbb{R}^n)$. Then $f(x)g(-i\nabla)$ is a bounded operator with singular values μ_m obeying

$$|\mu_m| \leq d_{q,n}\|f\|_q\|g\|_{q,w}m^{-1/q}$$

What we mean when we say that $f(x)g(-i\nabla)$ is in $\mathscr{I}_q$ is that there is an A in $\mathscr{I}_q$ so that

$$(\varphi, A\psi) = (\bar{f}\varphi, g(-i\nabla)\psi)$$

for all φ and ψ in $\mathscr{S}(\mathbb{R}^n)$.

We shall give proofs of Theorems XI.20 and XI.21; the reader can find a reference for Theorem XI.22 in the Notes. We note that Theorem XI.20 cannot be extended to any $q < 2$ (see Problem 36). Theorem XI.21 is closely

related to the $q \geq 2$ result since $f \in L^2_\delta(\mathbb{R}^n)$ for $\delta > n/2$ implies that $f \in L^1(\mathbb{R}^n)$, and moreover it is not a much stronger hypothesis than $f \in L^1(\mathbb{R}^n)$. Theorem XI.22 is also related to Theorem XI.20 in that $|\mu_m| \leq cm^{-1/q}$ says that $\sum |\mu_m|^q$ is convergent or only barely divergent so that $f(x)g(-i\nabla)$ is almost in $\mathscr{I}_q$. Theorem XI.22 cannot be extended to allow both f and g to lie in L^q_w. For example, the operator $|x|^{-\alpha}|i\nabla|^{-\alpha}$ is not even compact since it commutes with the unitary group of dilations.

Proof of Theorem XI.20 If $q = \infty$, then f and g are in L^∞ so $\|f(x)g(-i\nabla)\|_{\text{op}} \leq \|f\|_\infty \|g\|_\infty$. If $q = 2$, then $f(x)g(-i\nabla)$ is an integral operator with kernel $f(x)(2\pi)^{-n/2}\check{g}(x - y)$ (see Theorem IX.29), so $f(x)g(-i\nabla)$ is Hilbert–Schmidt and $\|f(x)g(-i\nabla)\|_2 \leq (2\pi)^{-n/2}\|f\|_2 \|g\|_2$. The general case now follows by applying the interpolation methods of the appendix to Section IX.4 (Problem 35). ∎

Proof of Theorem XI.21 Write

$$f(x)g(-i\nabla) = AB$$

where

$$A = f(x)(1 - \Delta)^{-\delta/2}(1 + x^2)^{\delta/2}$$

$$B = (1 + x^2)^{-\delta/2}(1 - \Delta)^{\delta/2}g(-i\nabla)$$

Then B is Hilbert–Schmidt by Theorem XI.20. Let h be $(2\pi)^{-n/2}$ times the Fourier transform of $(1 + k^2)^{-\delta/2}$. Then A is an integral operator with kernel $f(x)h(x - y)(1 + y^2)^{\delta/2}$. Since $f \in L^2_\delta$, in order to prove that A is Hilbert–Schmidt, we need only show that

$$\int (1 + y^2)^\delta |h(x - y)|^2 \, dy \leq c(1 + x^2)^\delta \tag{49}$$

Now, $(1 + k^2)^{-\delta/2}$ has an analytic continuation H to $\{z \mid |\text{Im } z| < 1\}$ which obeys $\int |H(k + i\kappa)|^2 \, dk < \infty$, so the Paley–Wiener principle (see Theorem IX.13) assures us that

$$\int e^{2a|x|} |h(x)|^2 \, dx < \infty$$

for all sufficiently small a. In particular,

$$\int (1 + x^2)^\delta |h(x)|^2 \, dx < \infty \tag{50}$$

Since $(1 + y^2)^\delta \leq 2^\delta(1 + |x - y|^2)^\delta(1 + x^2)^\delta$, (49) follows from (50). Thus, since A and B are both Hilbert–Schmidt, their product is trace class. ∎

Appendix 3 to XI.3: A general invariance principle for wave operators

In developing the Kato–Birman theory, a striking invariance principle (Theorem XI.11) for the wave operators appeared. One can ask whether this invariance principle holds under more general hypotheses than the condition that $A - B$ be trace class. Our goal in this appendix is to prove a similar result under a hypothesis of the type used in Cook's method.

Theorem XI.23 Let A and B be self-adjoint operators on a Hilbert space $\mathscr{H}$ and φ a function on a finite interval $(a, b) \subset \mathbb{R}$ such that:

(i) The distributional derivative φ'' is in L^1 and $\varphi'(x) \geq \alpha > 0$ for all $x \in (a, b)$.

(ii) Let I be a compact subinterval of (a, b). Let $\mathscr{D}$ be a dense subset of $E_I(B)P_{\text{ac}}(B)\mathscr{H}$ contained in $\mathscr{M}(B)$ such that for any $u \in \mathscr{D}$, the function

$$w(t) = e^{iAt}e^{-iBt}u$$

is strongly differentiable with $\|w'(t)\| \in L^1(\pm 1, \pm\infty) \cap L^2(\pm 1, \pm\infty)$ and $|t|^\alpha\|w'(t)\| \in L^1(\pm 1, \pm\infty)$ for some $\alpha > 0$.

Then, for any $u \in \mathscr{D}$,

$$\lim_{t \to \mp\infty} e^{i\varphi(A)t}e^{-i\varphi(B)t}u$$

exist and equal $\Omega^\pm(A, B)u$.

In particular, suppose that φ is an admissible function on an open set T with $\sigma(A), \sigma(B) \subset \bar{T}$ so that at each boundary point of T either φ has a finite limit or both A and B do not have point spectrum at that point. Then $\Omega^\pm(\varphi(A), \varphi(B))$ exist and

$$\Omega^\pm(\varphi(A), \varphi(B)) = \Omega^\pm(A, B)E_{T_1}(B) + \Omega^\mp(A, B)E_{T_2}(B)$$

where T_1 (respectively, T_2) is the union of those intervals where $\varphi' > 0$ (respectively, $\varphi' < 0$).

To prove this theorem, we need to develop a theory of Fourier transforms of (weakly) measurable $\mathscr{H}$-valued functions in $L^p(\mathbb{R}; \mathscr{H})$ $(p < \infty)$. The easiest way to define this is to let $\mathscr{S}(\mathbb{R}; \mathscr{H})$ denote the space of C^∞ functions from $\mathbb{R}$ to $\mathscr{H}$ with $\sup_\lambda \|(1 + |\lambda|)^n D^\alpha f(\lambda)\| < \infty$ for all α, n. The Fourier

transform is then defined as a *weak* integral (recall that all our vector-valued integrals in these volumes are weak integrals),

$$\hat{f}(k) = (2\pi)^{-1/2} \int e^{-ik\lambda} f(\lambda)\, d\lambda \tag{51}$$

By duality, one extends $\hat{}$ to $\mathscr{S}'(\mathbb{R}; \mathscr{H})$ and thus to $L^p(\mathbb{R}; \mathscr{H}) \subset \mathscr{S}'(\mathbb{R}; \mathscr{H})$. In particular, the Plancherel theorem holds. Indeed, realizing $L^2(\mathbb{R}; \mathscr{H})$ as $L^2(\mathbb{R}) \otimes \mathscr{H}$ as in Section II.4, our extended Fourier transform is just $\mathscr{F} \otimes 1$. Moreover, for $f \in L^1(\mathbb{R}; \mathscr{H})$, (51) holds pointwise.

Let $F \in L^1(\mathbb{R})$. Then, for any $v \in \mathscr{H}$, we claim that

$$\hat{F}(A)v = (2\pi)^{-1/2} \int F(\lambda) e^{-i\lambda A} v\, d\lambda \tag{52}$$

for any self-adjoint A. For (52) holds when $F \in \mathscr{S}(\mathbb{R})$ and so, by a limiting argument it holds for $F \in L^1$.

Fix a function $g \in C_0^\infty(a, b)$ so that $g = 1$ on I and $0 \le g \le 1$. Define

$$G(t, s) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} e^{is\eta - it\varphi(\eta)} g(\eta)\, d\eta$$

Lemma 1 Let φ satisfy hypothesis (i) of Theorem XI.23. Then:

(a) For each fixed t, $G(t, \cdot) \in L^1(\mathbb{R})$.
(b) For each fixed s, $G(t, s) \to 0$ as $t \to \pm\infty$.
(c) $c(t)^2 \equiv \int_{-\infty}^{0} |G(t, s)|^2\, ds \to 0$ as $t \to \infty$.
(d) For $v \in \mathscr{H}$ and self-adjoint A,

$$(2\pi)^{-1/2} \int_{-\infty}^{\infty} G(t, s) e^{-isA} v\, ds = e^{-it\varphi(A)} g(A) v$$

Proof (a) For each fixed t, $G(t, \cdot)$ is the Fourier transform of a function of compact support with second derivatives in L^1. Thus $(1 + t^2)G(t, \cdot) \in L^\infty$ so that $G(t, \cdot)$ is certainly in L^1.

(b) Clearly, $|G(t, s)| \le (2\pi)^{-1/2} \|g\|_1$, so it suffices to prove (b) for a g that is a sum of functions of the form $e^{-is\eta} \chi_\Omega(\eta) \varphi'(\eta)$ which are dense in $L^1(I)$. For such g's the result is easy.

(c) is just a restatement of Lemma 3b of Section 3 and (d) follows from (52). ∎

Lemma 2 Let $h \in \mathscr{S}'(\mathbb{R}; \mathscr{H})$ have a Fourier transform in $L^1(\mathbb{R}; \mathscr{H})$ and let C be self-adjoint. Let $G(t, s)$ be as in Lemma 1. Then the integral

$$J_h(t) \equiv \int_{-\infty}^{\infty} G(t, s) e^{-isC} h(s)\, ds$$

exists and

$$\lim_{t \to \pm\infty} \|J_h(t)\| = 0 \tag{53}$$

Proof Since $\hat{h} \in L^1$, h is in L^∞ so the integral exists by Lemma 1a. Let $v \in \mathscr{H}$. Then

$$(v, J_h(t)) = \int_{-\infty}^{\infty} (\overline{G(t, s)} e^{+isC} v, h(s))\, ds$$

$$= \int (e^{it\varphi(C-k)} g(C - k)v, \hat{h}(k))\, dk$$

on account of the Plancherel theorem and Lemma 1d. Thus

$$\|J_h(t)\| \le \|\hat{h}\|_{L^1} \tag{54}$$

By (54), it suffices to show that (53) holds for a total subset of $\hat{h}$ in L^1, so we consider the case $\hat{h}(k) = f(k)u; f \in C_0^\infty(\mathbb{R})$, $u \in \mathscr{H}$. In that case

$$J_h(t) = F_t(C)u$$

where

$$F_t(s) = \int f(k) e^{-it\varphi(s-k)} g(s - k)\, dk$$

Now, $\|F_t\|_\infty \le \|f\|_1$ for all t, and for each fixed s, $F_t(s) \to 0$ as $t \to \pm\infty$ by Lemma 1b. Thus, by Theorem VII.2d, s-$\lim_{t \to \pm\infty} F_t(C) = 0$, so the lemma is proven. ∎

Lemma 3 Let $h(t)$ be a strongly differentiable function from $\mathbb{R}$ to $\mathscr{H}$ and suppose that:

(i) $\|h(t)\| \to 0$ as $t \to \infty$.
(ii) $\|h'(t)\| \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$.
(iii) $|t|^\alpha \|h'(t)\| \in L^1(\mathbb{R})$ for some $\alpha > 0$.

Then $\hat{h} \in L^1(\mathbb{R}; \mathscr{H})$.

Proof Let G be the Fourier transform of h'. Then by (ii) and (iii), $G \in L^1 \cap L^2$ and

$$\|G(k) - G(\ell)\| \leq c_\theta |k - \ell|^\theta$$

for $\theta = \min\{\alpha, 1\}$. By (i),

$$\begin{aligned}\int (v, h'(t))\, dt &= \lim_{a\to\infty} \int_{-a}^{a} (v, h'(t))\, dt \\ &= \lim_{a\to\infty} [(v, h(a)) - (v, h(-a))] = 0\end{aligned}$$

so $G(0) = 0$. It follows that $\|G(k)\| \leq c|k|^\theta$. Now let $K(k) = (ik)^{-1}G(k)$. Then $\int_{|k|\geq 1} |K(k)|\, dk < \infty$ since k^{-1} and G are both in $L^2(\pm 1, \pm\infty)$. Moreover, $\int_{-1}^{1} |K(k)|\, dk < \infty$ since $|K(k)| \leq C|k|^{\theta-1}$.

We shall be finished if we prove that $\check{K} = h$. But $\check{K}$ and h have the same derivative, so $\check{K} = h + v$ for some constant vector v. Since $K \in L^1$, $\check{K}(t) \to 0$ as $t \to \infty$ by the Riemann–Lebesgue lemma, so, using hypothesis (i), $v = 0$. ∎

Proof of Theorem XI.23 Fix $u \in \mathscr{D}$ and let

$$I(t) = e^{-it\varphi(A)}\Omega^- u - e^{-it\varphi(B)}u$$

We must show that $I(t) \to 0$ as $t \to \infty$. Let $w(t) = e^{iAt}e^{-iBt}u$ and $w_- = \Omega^- u$. Then, by Lemma 1d and the fact that $g(B)u = u$, and $g(A)\Omega^- u = \Omega^- g(B)u = \Omega^- u$,

$$I(t) = (2\pi)^{-1/2} \int G(t, s)e^{-isA}[w_- - w(s)]\, ds$$

Fix positive C^∞ functions K_0 and $K_\pm$ such that $K_0 \in C_0^\infty$, supp $K_\pm \subset [\pm 1, \pm\infty)$, and $K_+ + K_- + K_0 = (2\pi)^{-1/2}$. Then $I(t) = \sum_{j=1}^4 I_j(t)$ where

$$I_j(t) = \int K_{\alpha(j)}(s)G(t, s)e^{-isA}[w_- - w(s)]\, ds$$

for $j = 1, 2$ and $\alpha(1) = 0$, $\alpha(2) = +$,

$$I_3(t) = \int K_-(s)G(t, s)e^{-isA}[w_+ - w(s)]\, ds$$

$$I_4(t) = \int K_-(s)G(t, s)e^{-isA}[w_- - w_+]\, ds$$

with $w_+ = \Omega^+ u$. By the hypotheses, Lemma 2, and Lemma 3, $I_2(t)$ and $I_3(t)$ go to zero as $t \to \infty$. Since

$$|I_1(t)| \leq 2\|u\|(2\pi)^{-1/2} \int_{\text{supp } K_0} |G(t, s)|\, ds$$

$I_1(t) \to 0$ as $t \to \infty$ on account of $|G(t, s)| \leq (2\pi)^{-1/2}\|g\|_1$, Lemma 1b and the dominated convergence theorem.

It remains to prove that $I_4(t) \to 0$ as $t \to \infty$. Now, by Lemma 1 in Section 3,

$$\int_{-\infty}^{\infty} |(v, e^{-isB}u)|^2\, ds \leq 2\pi\|\|u\|\|^2\|v\|^2$$

Thus,

$$\begin{aligned}\int_{-\infty}^{\infty} |(v, e^{-isA}w_\pm)|^2\, ds &\leq \int_{-\infty}^{\infty} |((\Omega^\pm)^* v, e^{-isB}u)|^2\, ds \\ &\leq 2\pi\|v\|^2\|\|u\|\|^2\end{aligned}$$

It follows that

$$\int |K_-(s)|^2 |(v, e^{-isA}(w_- - w_+))|^2\, ds \leq \text{const}\|v\|^2$$

so that $|I_4(t)| \leq \text{const}\, c(t)$ where $c(t)$ is given in Lemma 1c. By that lemma, $I_4(t) \to 0$. ∎

In most cases where one really needs the invariance of the wave operators (see Example 1 (revisited) in Section 10 or Example 4 in Section 11), one has already satisfied the hypotheses of the Kato–Birman theory which has the invariance of the wave operators as a corollary. Nevertheless, Theorem XI.23 is interesting since it shows that the invariance principle can hold even when there is no information about asymptotic completeness.

Example 1 Suppose that the hypotheses of Theorem XI.16 hold with (45) replaced by the stronger assumption

$$\int_{+1}^{\infty} t^\alpha \left(\int_{a<|x|<b} |V(xt)|^2\, dx \right)^{1/2} dt < \infty$$

In particular, this will be true if $|V(x)| \leq c|x|^{-1-\varepsilon}$ near ∞. Then $\Omega^\pm(H^2, H_0^2)$ exist.

Example 2 We want to apply the invariance principle to show the absence of relativistic corrections for electron scattering from external (not necessarily constant) magnetic fields, at least in the approximation that the electron magnetic moment is $e\hbar/mc$ (the physical value differs from this by about 1% due to corrections attributed to quantum electrodynamics). In units with $\hbar = c = 1$, the nonrelativistic Schrödinger Hamiltonian is

$$H_S(A) = \frac{(p - eA)^2}{2m} + \frac{e}{2m}(\sigma \cdot B)$$

acting on $L^2(\mathbb{R}^3; \mathbb{C}^2)$ where, as usual, $p = -i$ grad. Here σ stands for the vector of Pauli spin matrices

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_2 = \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}, \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

A is the magnetic vector potential and $B = \text{curl } A$. The relativistic theory is described by the Dirac Hamiltonian

$$H_D(A) = \alpha \cdot (p - eA) + m\beta$$

acting on $L^2(\mathbb{R}^2; \mathbb{C}^4)$. If $\mathbb{C}^4$ is realized as $\mathbb{C}^2 \otimes \mathbb{C}^2$, the conventional choice for α, β is

$$\alpha_i = \sigma_1 \otimes \sigma_i, \qquad \beta = \sigma_3 \otimes 1$$

A direct and elementary formal calculation shows that

$$1 \otimes H_S(A) = (2m)^{-1}[H_D^2(A) - m^2]$$

If A is C^1, with both A and ∇A bounded, then this formal calculation is certainly an equality on the level of self-adjoint operators. If, moreover, $|A(r)| \leq C(1 + r)^{-1-\epsilon}$, then $\Omega^{\pm}(H_D(A), H_D(0))$ exists by a stationary phase analysis. Moreover, the invariance principle, Theorem XI.23, is applicable, so

$$\Omega^{\pm}(H_D(A), H_D(0)) = 1 \otimes \Omega^{\pm}(H_S(A), H_S(0))$$

This demonstrates the absence of relativistic corrections to scattering at least if the scattering is described in terms of position or momentum variables. Of course, if asymptotic velocities or energies are used, one must remember to use the appropriate kinematics.

XI.4 Quantum scattering I: Two-body case

The scattering theory that we shall study in the most detail is scattering for two-body quantum systems or, what is equivalent, a one-body system in an external potential. This is the most thoroughly studied field in scattering theory, and there is a wide variety of interesting results.

The Hilbert space of a two-particle system is

$$\mathscr{H} = L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3) = L^2(\mathbb{R}^6)$$

The free Hamiltonian is

$$\tilde{H}_0 = -\frac{1}{2\mu_1}\Delta_1 - \frac{1}{2\mu_2}\Delta_2$$

where $\mathbf{r} \in \mathbb{R}^6$ is written $\mathbf{r} = \langle \mathbf{r}_1, \mathbf{r}_2 \rangle$ with $\mathbf{r}_i \in \mathbb{R}^3$ and Δ_i is the three-dimensional Laplacian associated to $\mathbf{r}_i$. The interacting Hamiltonian is

$$\tilde{H} = \tilde{H}_0 + V(\mathbf{r}_1 - \mathbf{r}_2)$$

where V is a function in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Thus Kato's theorem (Theorem X.16) shows that $\tilde{H}$ is self-adjoint on $C_0^\infty(\mathbb{R}^6)$. We shall later place more severe restrictions on V.

First, we change coordinates to separate the center of mass motion. The new coordinates will be

$$\mathbf{R} = (\mu_1 + \mu_2)^{-1}(\mu_1\mathbf{r}_1 + \mu_2\mathbf{r}_2), \qquad \mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$$

Let U be the unitary operator on $L^2(\mathbb{R}^6)$ given by

$$(Uf)(\mathbf{x}, \mathbf{y}) = f((\mu_1 + \mu_2)^{-1}(\mu_1\mathbf{x} + \mu_2\mathbf{y}), \mathbf{x} - \mathbf{y})$$

and let $\mathbf{r}_1$ and $\mathbf{r}_2$ denote the obvious coordinate multiplication operators. Denote $U\mathbf{r}_1U^{-1}$ by $\mathbf{R}$ and $U\mathbf{r}_2U^{-1}$ by $\mathbf{r}_{12}$. Then

$$U\tilde{H}U^{-1} = -\frac{1}{2(\mu_1 + \mu_2)}\Delta_{\mathbf{R}} - \frac{1}{2m}\Delta_{r_{12}} + V(\mathbf{r}_{12})$$

$$U\tilde{H}_0U^{-1} = -\frac{1}{2(\mu_1 + \mu_2)}\Delta_{\mathbf{R}} - \frac{1}{2m}\Delta_{r_{12}}$$

where $m^{-1} = \mu_1^{-1} + \mu_2^{-1}$ (Problem 40). We now write $L^2(\mathbb{R}^6) = L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$ where now the variables are $\mathbf{R}$ and $\mathbf{r}_{12}$. Then, as operators on $\tilde{D} \equiv C_0^\infty(\mathbb{R}^3) \otimes C_0^\infty(\mathbb{R}^3) \subset C_0^\infty(\mathbb{R}^6)$, $U\tilde{H}_0U^{-1}$ and $U\tilde{H}U^{-1}$ can be decomposed as

$$U\tilde{H}_0U^{-1} = h_0 \otimes I + I \otimes H_0$$

$$U\tilde{H}U^{-1} = h_0 \otimes I + I \otimes H$$

where

$$h_0 = -[2\mu_1 + 2\mu_2]^{-1}\Delta$$

$$H_0 = -(2m)^{-1}\Delta$$

$$H = -(2m)^{-1}\Delta + V(r)$$

Thus, $e^{-itUH_0U^{-1}} = e^{-ith_0} \otimes e^{-itH_0}$ and $e^{-itUHU^{-1}} = e^{-ith_0} \otimes e^{-itH}$. Since these differ only in the second factor, we shall define wave operators $\Omega^{\pm}$ and a scattering operator S for the system $\{e^{-itH}, e^{-itH_0}\}$ on $L^2(\mathbb{R}^3)$. The wave and scattering operators for the original system are then given by $U^{-1}(I \otimes \Omega^{\pm})U$ and $U^{-1}(I \otimes S)U$.

The description we have just given of the coordinate change in terms of a unitary operator is the so-called "active" way of looking at a coordinate transformation. There is a second way of looking at the transformation—the so-called "passive" way. In this interpretation, we think of $-\Delta_1 - \Delta_2$ and $-\frac{1}{2}\Delta_{\mathbf{R}} - 2\Delta_{r12}$ as the *same* operator (rather than as unitarily equivalent operators) written in terms of a different basic set of coordinates. When there are several coordinate changes, as we shall encounter in Section 6, this second "passive" viewpoint is notationally less cumbersome than the first "active" viewpoint. We shall henceforth adopt this second "passive" viewpoint.

Given our discussion in the preceding section, it is clear that the existence of scattering states is equivalent to the existence of $\Omega^{\pm}(H, H_0)$. Notice that the uniqueness of scattering states is trivial, for if both $\|e^{-iHt}\psi_1 - e^{-itH_0}\varphi\|$ and $\|e^{-iHt}\psi_2 - e^{-itH_0}\varphi\|$ go to zero as $t \to -\infty$, then $\psi_1 - \psi_2 = 0$ by the linearity and uniform boundedness of e^{-iHt}.

The basic existence result is the following:

Theorem XI.24 (the Cook–Hack theorem) Let $V \in L^2(\mathbb{R}^3) + L^r(\mathbb{R}^3)$ for $2 \le r < 3$. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and let $H = H_0 + V$. Then $\Omega^{\pm}(H, H_0)$ exist.

We shall give three different proofs, all based on Cook's method, which illustrate the variety of ways one can estimate $\|Ve^{-itH_0}\varphi\|$.

First proof of Theorem XI.24 This is the most "elementary" proof in that it involves only direct calculations and does not require either interpolation or stationary phase ideas. Fix $\gamma > 0$ and let

$$\varphi_\gamma(x) = \gamma^{3/4} \exp(-\tfrac{1}{2}\gamma x^2)$$

Then, we have that

$$(e^{-itH_0}\varphi_\gamma)(x) = \alpha(t)^{3/4} \exp(-\tfrac{1}{2}[\alpha(t) + i\beta(t)]x^2) \tag{55}$$

where $\beta(t)$ is a suitable real-valued function and

$$\alpha(t) = \gamma(1 + 4t^2\gamma^2)^{-1}$$

To prove (55) one need only note that, up to a constant, $\hat{\varphi}_\gamma$ is $\exp(-\frac{1}{2}p^2/\gamma)$ so that $(e^{-itH_0}\varphi_\gamma)\hat{}$ is $\exp(-\frac{1}{2}p^2/(\gamma(t))$ where $\gamma(t)^{-1} = \gamma^{-1} - 2it$. (55) then follows where the constant can be evaluated by using $\|e^{-itH_0}\varphi_\gamma\|_2 = \|\varphi_\gamma\|_2$.

From (55) one easily sees (Problem 42) that for $k > 0$,

$$\|(1 + |x|)^k e^{-itH_0}\varphi_\gamma\|_\infty \le c(1 + |t|)^{-\frac{3}{2}+k} \tag{56}$$

It follows that

$$\begin{aligned}\|Ve^{-itH_0}\varphi_\gamma\|_2 &\le c\|(1 + |x|)^{-k}V\|_2(1 + |t|)^{-\frac{3}{2}+k} \\ &\le c'(\|V_2\|_2 + \|V_r\|_r)(1 + |t|)^{-\frac{3}{2}+k}\end{aligned}$$

if $V = V_2 + V_r \in L^2 + L^r$ and $r^{-1} = \frac{1}{2} + k/(3 + \varepsilon)^{-1}$ for some $\varepsilon > 0$. This follows from Hölder's inequality and the fact that $(1 + |x|)^{-k} \in L^m$ for all $m > 3k^{-1}$. Since $r < 3$, we can take $k < \frac{1}{2}$, so

$$\int \|Ve^{-itH_0}\varphi_\gamma\|_2 \, dt < \infty$$

for any γ. Since linear combinations of translates of the φ_γ are dense (Problem 43), this estimate and Cook's method (Theorem XI.4) imply that $\Omega^{\pm}(H, H_0)$ exist. ∎

Second proof of Theorem XI.24 By Cook's method we need only show that for any $\varphi \in \mathscr{S}$, $f(t) = \|Ve^{-itH_0}\varphi\|_2$ is in $L^1(1, \infty)$. Recall Theorem IX.30, which says that

$$\|e^{-iH_0t}\varphi\|_p \le t^{-\frac{3}{2}+3/p}\|\varphi\|_q$$

if $\varphi \in \mathscr{S}$ and $q^{-1} = 1 - p^{-1}$, $2 \le p \le \infty$. Write $V = V_2 + V_r$ where $V_2 \in L^2$, $V_r \in L^r$ and let $p^{-1} = \frac{1}{2} - r^{-1}$ so $p > 6$. Then, by Hölder's inequality,

$$\begin{aligned}\|Ve^{-iH_0t}\varphi\|_2 &\le \|V_2\|_2\|e^{-iH_0t}\varphi\|_\infty + \|V_r\|_r\|e^{-iH_0t}\varphi\|_p \\ &\le \|V_2\|_2\|\varphi\|_1 t^{-\frac{3}{2}} + \|V_r\|_r\|\varphi\|_q t^{-\frac{3}{2}+3/p}\end{aligned}$$

Since $p > 6$, $\frac{3}{2} - 3p^{-1} > 1$ so $f(t) \in L^1(1, \infty)$ which proves the theorem. ∎

Notice that the condition $r < 3$ was crucial since it implied $p > 6$ and the $t^{-\alpha}$ decay with $\alpha > 1$ which is necessary for $f(t)$ to be in $L^1(1, \infty)$. Which $(1 + |r|)^{-\beta}$ potentials are in $L^2 + L^r$? Precisely those with $\beta > 1$. Again, as in the classical case, simple scattering theory breaks down at the Coulomb force. We shall discuss how to modify quantum scattering theory to handle the Coulomb case in Section 9.

Third proof of Theorem XI.24 By Theorem XI.16, it suffices to prove that (45) holds since we can then use stationary phase estimates. Write

$V = V_2 + V_r$ with $V_2 \in L^2$ and $V_r \in L^r$. By Hölder's inequality,

$$\left(\int_{at<|x|<bt} |V_r(x)|^2\,dx\right)^{\frac{1}{2}} \leq \|V_r\|_r \left(\int_{at<|x|<bt} dx\right)^{\frac{1}{2}-1/r}$$
$$= C\|V_r\|_r t^{\frac{1}{2}-3/r}$$

Thus,

$$\int_1^\infty \left(\int_{a<|x|<b} |V_r(xt)|^2\,dx\right)^{\frac{1}{2}} dt \leq \int_1^\infty Ct^{-3/r}\|V_r\|_r\,dt < \infty$$

since $r < 3$. Since $|V(x)|^2 \leq 2|V_2(x)|^2 + 2|V_r(x)|^2$, (45) holds. ∎

This result can be extended in various directions. If $\mathbb{R}^3$ is replaced by $\mathbb{R}^n$ and $n > 3$, then one can see that the theorem holds if the condition $r < 3$ is replaced by $r < n$; all of the above proofs extend. Of course for general $V \in L^2 + L^r$ it may happen that $H_0 + V$ is not essentially self-adjoint on C_0^∞; the arguments work for *any* self-adjoint extension of $(H_0 + V) \upharpoonright C_0^\infty$. When $V \in L^{n/2} + L^r$ $(n \geq 5)$ or $L^{2+\varepsilon} + L^r$ $(n = 4)$, we know that $H_0 + V$ is self-adjoint on $D(H_0)$ by general principles. For $n = 1$ or 2, only the third proof extends; the result appears in Problem 44. A second direction for extension allows local singularities:

Theorem XI.25 Let V be a measurable function on $\mathbb{R}^3$ so that there is an R, an $\varepsilon > 0$, and a C with

$$|V(\mathbf{r})| \leq Cr^{-1-\varepsilon} \quad \text{if} \quad r > R$$

Let H be an operator with the property that $D_R \equiv C_0^\infty(\mathbb{R}^3 \backslash \{\mathbf{r} \mid r < R\}) \subset D(H)$, H is self-adjoint, and

$$H\varphi = -\Delta\varphi + V\varphi$$

for $\varphi \in D_R$. Let $H_0 = -\Delta$. Then $\Omega^\pm(H, H_0)$ exist.

Proof Let χ be the operator of multiplication by a function in C_0^∞ that is one on the ball of radius R. Then, as in the proof of the Cook–Hack theorem,

$$\|[H(1-\chi) - (1-\chi)H_0]e^{-itH_0}\varphi\| \in L^1$$

since $H(1-\chi) - (1-\chi)H_0 = V(1-\chi) - \Delta\chi - \nabla\chi \cdot \text{grad}$ and

$$\text{grad}(e^{-itH_0}\varphi) = e^{-itH_0}(\text{grad}\,\varphi).$$

Moreover, $\chi(H_0 + 1)^{-1}$ is Hilbert–Schmidt and so compact. By Problem 18, this implies that $\lim_{t\to\infty} \|\chi e^{-itH_0}\varphi\| = 0$. The result now follows from the Kupsch–Sandhas theorem (Theorem XI.5). ∎

Since one has an explicit formula for $e^{-itH_0}\varphi$, one can prove directly that $\lim_{t\to\infty} \|\chi e^{-itH_0}\varphi\| = 0$ without appealing to the abstract result in Problem 18.

Finally, there are quadratic form results.

Theorem XI.26 Let $V = V_1 + V_2$ be a function on $\mathbb{R}^3$ so that $W_1 \equiv (1 + |x|^2)^{\frac{1}{2}+\varepsilon}V_1$ is in $L^\infty + L^\infty$ and V_2 is in $L^\infty \cap L^{\frac{1}{2}-\delta}$ for some $\varepsilon > 0$ and $\delta > 0$. Let $H_0 = -\Delta$ and $H = H_0 + V$ as a quadratic form sum. Then $\Omega^\pm(H, H_0)$ exist.

Proof Write $V = C_1 D_1 + C_2 D_2$ with $C_1^* = W_1/|W_1|^{\frac{1}{2}}$,

$$D_1 = |W_1|^{\frac{1}{2}}(1 + |x|^2)^{-\frac{1}{2}-\varepsilon},$$

$C_2^* = V_2/|V_2|^{\frac{1}{2}}$ and $D_2 = |V_2|^{\frac{1}{2}}$. Then by hypothesis, $C_1^*C_1$, $D_1^*D_1$, $C_2^*C_2$, and $D_2^*D_2$ are all H_0-form bounded with relative bound zero, so, by Theorem XI.6, it suffices to prove that for $\varphi \in \mathscr{S}(\mathbb{R}^3)$ we have $\|D_1 e^{-itH_0}\varphi\| \in L^1$ and $\|D_2 e^{-itH_0}\varphi\| \in L^1$. Since $D_2 \in L^{3-2\delta}$, the second expression is in L^1 by the proof of Theorem XI.24. Let $f = (1 + |x|^2)^{-\frac{1}{2}-\varepsilon}$. Then since $D_1(H_0 + 1)^{-1}$ is bounded, it suffices to show that $G(t) \equiv \|(H_0 + 1)fe^{-itH_0}\varphi\|$ is in L^1.

$$(H_0 + 1)fe^{-itH_0}\varphi$$
$$= fe^{-itH_0}[(H_0 + 1)\varphi] - 2(\nabla f)e^{-itH_0}(\text{grad}\,\varphi) - (\Delta f)e^{-itH_0}\varphi$$

Since φ, $(H_0 + 1)\varphi$, grad φ are in $\mathscr{S}$ and f, ∇f, $-\Delta f$ are in $L^2 + L^{3-\varepsilon}$, we conclude that $G \in L^1$. ∎

We shall prove in Section XIII.4 that for $V \in L^{3/2} + (L^\infty)_\varepsilon$, $\sigma_{\text{ess}}(-\Delta + V) = [0, \infty)$. Since $\sigma_{\text{ac}} \subset \sigma_{\text{ess}}$, we have

Corollary The operator H of Theorem XI.26 obeys $\sigma_{\text{ac}}(H) = [0, \infty)$.

The methods we have developed work for other cases than the pairs $H = -\Delta + V$, $H_0 = -\Delta$. Consider the case $B_0 = -\Delta + x_1$, $B = -\Delta + V + x_1$, where x_1 is the first component of $\mathbf{x}$. This pair describes scattering in a constant external electric field. As a preliminary, we need:

Lemma Let $B_0 = -\Delta + x_1$. Then

$$e^{-itB_0} = e^{-itx_1}e^{-it^3/3}e^{+it^2p_1}e^{-itH_0}$$

where $H_0 = -\Delta$.

Proof Consider first the one-dimensional case. Let $f(\alpha) = e^{ip^3\alpha}xe^{-ip^3\alpha}$. Then, as an operator from $\mathscr{S}(\mathbb{R})$ to itself, $f(0) = x$ and $f'(\alpha) = 3p^2$. Thus $f(\alpha) = x + 3p^2\alpha$. It follows that for each α, $f(\alpha)$ is essentially self-adjoint on $\mathscr{S}(R)$, and for any bounded Borel function

$$F(x + 3p^2\alpha) = e^{ip^3\alpha}F(x)e^{-ip^3\alpha}$$

Thus

$$\begin{aligned} e^{-it(p^2+x)} &= e^{ip^3/3}e^{-itx}e^{-ip^3/3} \\ &= e^{-itx}e^{i(p-t)^3/3}e^{-ip^3/3} \\ &= e^{-itx}e^{-it^3/3}e^{it^2p}e^{-itp^2} \end{aligned}$$

where in the second step we used $e^{itx}g(p)e^{-itx} = g(p - t)$. In the n-dimensional case, let $\mathbf{p} = \langle p_1, \mathbf{p}_\perp \rangle$. Then

$$e^{-itB_0} = e^{-it(p_1^2+x_1)}e^{-itp_\perp^2}$$

So, by the one-dimensional case, the result holds. ∎

Theorem XI.27 (the Avron–Herbst theorem) Let $\mathbf{x} = \langle x_1, \mathbf{x}_\perp \rangle$. Let V be a function on $\mathbb{R}^n$ obeying:

(i) $\displaystyle\int_{|y-x|\le 1} |V(y)|^2\, dy \le C(1 + |x|^2)^N$

for some N and C and *all* x.

(ii) For some k and ℓ with $2\ell - k > 1$ and some x_0,

$$\left(\int_{|y-x|\le 1} |V(y)|^2\, dy\right)^{\frac{1}{2}} \le C(1 + |x_\perp|)^k/(1 + |x_1|)^\ell$$

for all x with $x_1 < -x_0$.

Let $B_0 = -\Delta + x_1$ and let B be some self-adjoint extension of $(B_0 + V) \upharpoonright \mathscr{S}(\mathbb{R}^n)$. Then $\Omega^\pm(B, B_0)$ exist.

Proof By the lemma, for $\varphi \in \mathscr{S}$,

$$\|Ve^{-itB_0}\varphi\|_2^2 = \int |V(x_1 - t^2, x_\perp)|^2\, |(e^{-itH_0}\varphi)(x)|^2\, dx$$

Thus by the stationary phase method we only need that, for any a and b bigger than zero, there is a T_0 with

$$\int_{T_0}^{\infty}\left(\int_{at\le|x|\le bt} |V(x_1 - t^2, x_\perp)|^2\, d^nx\right)^{\frac{1}{2}} t^{-n/2}\, dt < \infty \qquad (57)$$

where we have used hypothesis (i) to control the integral over the remaining x. (57) follows easily from hypothesis (ii). ∎

We emphasize that only x_1 very negative is involved in hypothesis (ii). Physically, this is because B_0 pushes the particle out to negative x_1. As an example, if $B = -\Delta - |x_1|$, then $\Omega^\pm(B, -\Delta - x_1)$ and $\Omega^\pm(B, -\Delta + x_1)$ both exist. Obviously, neither is complete by itself.

* * *

The idea of wave operators and Cook's method for proving their existence is also applicable to a variety of time-dependent quantum-mechanical situations. Thus, consider solutions of a time-dependent Schrödinger equation

$$i\frac{d}{dt}\psi(t) = H(t)\psi(t)$$

where we have in mind $H(t) = -\Delta + V(t)$, and each $V(t)$ is multiplication by a real function. In Section X.12 we discussed the solution of this equation and found, under suitable hypotheses, that there exists a strongly continuous two-parameter family of unitaries $U(t, s)$ obeying

$$U(t, s)U(s, v) = U(t, v), \qquad U(s, s) = 1$$

$$\frac{d}{dt}[U(t, s)\psi] = -iH(t)U(t, s)\psi, \qquad \psi \in D(H_0)$$

See Theorem X.71. A simple case where one is certain that solutions of $U(t, 0)\psi$ should exist which asymptotically look like $e^{-itH}\psi$ is when $V(t) = V_1 + \varphi(t)V_2$ where φ has compact support and say $V_1, V_2 \in L^2(\mathbb{R}^3)$; in fact using the existence of the limit of $e^{i(H_0+V_1)t}e^{-iH_0t}$ as $t \to \pm\infty$, it is easy to prove that suitable "time-dependent" wave operators exist in this case. Actually, such wave operators exist under very general circumstances, for example, if

$$V(t) = (\cos \omega_1 t)V_1 + (\cos \omega_2 t)V_2$$

At first sight this may seem surprising, for why should $U(t, 0)\psi$ have a simple limit when $H(t)$ continues to oscillate? The reason is simple: Scattering states spread out as $t \to \pm\infty$, so it does not matter what the potential is doing locally so long as it goes to zero at ∞.

Definition Let $U(t, s)$ be the unitary propagator associated to $H(t) = H_0 + V(t)$ according to Theorems X.70 and X.71. We say that the associated wave operators exist if and only if

$$\Omega^{\pm} \equiv \underset{t \to \mp\infty}{\text{s-lim}}\, U(t, 0)^* e^{-iH_0 t} \tag{58}$$

exist.

Theorem XI.28 Let $V(t) = V_1(t) + V_2(t)$, where $V_1(t)$ is a strongly differentiable $L^2(\mathbb{R}^3)$-valued function and $V_2(t)$ is a strongly differentiable $L^p(\mathbb{R}^3)$-valued function, $2 \le p \le \infty$. Suppose that for some $\varepsilon > 0$ and suitable c,

$$\|V_1(t)\|_2 \le c\,|t|^{-\frac{1}{2}-\varepsilon}, \qquad |t| \ge 1$$
$$\|V_2(t)\|_p \le c\,|t|^{-\frac{1}{2}-3p^{-1}-\varepsilon}, \qquad |t| \ge 1$$

Then the limits (58) exist.

Proof Let $\varphi, \psi \in \mathscr{S}(\mathbb{R}^3)$. Then, by Theorem X.71,

$$\frac{d}{dt}(\varphi, U(t, 0)^* e^{-iH_0 t}\psi) = \frac{d}{dt}(U(t, 0)\varphi, e^{-iH_0 t}\psi)$$
$$= i(\varphi, U(t, 0)^* V(t) e^{-iH_0 t}\psi)$$

It follows that for $t > s$,

$$\|U(t, 0)^* e^{-iH_0 t}\psi - U(s, 0)^* e^{-iH_0 s}\psi\| \le \int_s^t \|V(u)e^{-iH_0 u}\psi\|\, du$$

By the hypotheses and the estimates in the second proof of Theorem XI.24, the last integral is convergent. Following Cook's method, we obtain the existence of the limit (58). ∎

Notice the striking feature of Theorem XI.28 in that it allows $V(t)$ to grow as $t \to \infty$! Using stationary phase ideas (Problem 45), one can show that for $V \in L^2$ *with compact support*, $V(t) = \varphi(t)V$ yields wave operators so long as φ is differentiable and of no more than polynomial growth at infinity.

The intertwining relations $e^{-iHs}\Omega^{\pm} = \Omega^{\pm} e^{-iH_0 s}$ do not, in general, have an analogue in the time-dependent case since $U(t + s, t)$ will not generally have a nice limit as $t \to \infty$. However, there is one special case of particular physical interest where there are still some intertwining relations.

Theorem XI.29 Let $V(t)$ obey the hypotheses of Theorem XI.28. Suppose, moreover, that $V(t + T) = V(t)$ for some fixed T and *all* $t \in \mathbb{R}$. Then

$$U(T, 0)\Omega^{\pm} = \Omega^{\pm} e^{-iH_0 T} \tag{59}$$

and in particular $e^{-iH_0 T}$ commutes with the scattering operator $(\Omega^-)^*\Omega^+$.

Proof Under the hypothesis, $U(t + T, s + T) = U(t, s)$, so that $U(nT, 0) = U(T, 0)^n$. Thus

$$U(nT, 0)^* e^{-iH_0(n+1)T} = U(T, 0)U((n + 1)T, 0)^* e^{-iH_0(n+1)T}$$

Taking $n \to \infty$, (59) results. ∎

Reintroducing $\hbar$ and letting $\omega = 2\pi/T$, one finds that Theorem XI.29 asserts that while H_0 may not be conserved by scattering, the energy can be changed only by $n\hbar\omega$ where $n = 0, \pm 1, \ldots$. This is a nonrelativistic justification of Planck's original quantization rule!

Much of the scattering theory we shall develop in this volume can be extended to the time-dependent case; we shall seldom do so explicitly in the text, but will give references in the Notes.

* * *

We now return to the basic quantum-mechanical problem of $\Omega^{\pm}(H, H_0)$ with $H_0 = -\Delta$. Completeness of these operators is easily handled with the Kato–Birman theory if V has sufficiently rapid falloff and sufficient local regularity. We shall later give an example where completeness is destroyed by severe local singularities.

Theorem XI.30 Let V be a measurable function on $\mathbb{R}^n$ so that $|V|$ is $-\Delta$-form bounded with relative bound $\alpha < 1$. Define $H = -\Delta + V$ as a form sum and let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$. If $V \in L^1(\mathbb{R}^n)$, then $\Omega^{\pm}(H, H_0)$ exist and are complete.

Proof We shall apply Birman's theorem (Theorem XI.10). Since $Q(H) = Q(H_0)$, the operators are mutually subordinate. Thus it suffices to show that $|V|^{\frac{1}{2}}E_I(H_0)$ and $E_I(H)|V|^{\frac{1}{2}}$ are both Hilbert-Schmidt. This follows if we show that $|V|^{\frac{1}{2}}(H_0 + E)^{-m}$ and $|V|^{\frac{1}{2}}(H + E)^{-m}$ are Hilbert-Schmidt for some m and E. By hypothesis, $|V|^{\frac{1}{2}} \in L^2$, so the first of these is Hilbert-Schmidt by Theorem XI.20 so long as $m > \frac{1}{4}n$. By mimicking the proof of

Theorem XI.12, $|V|^{\frac{1}{2}}(H+E)^{-m}$ is also Hilbert-Schmidt: explicitly by interpolation between $(H_0+E)^{-\frac{1}{2}}V(H_0+E)^{-m-\frac{1}{2}} \in \mathscr{I}_2$ and

$$\gamma \equiv \|(H_0+E)^{-\frac{1}{2}}V(H_0+E)^{-\frac{1}{2}}\| < \infty,$$

we see that $|V|^{\frac{1}{2}}(H_0+E)^{-k-\frac{1}{2}}$ and $(H_0+E)^{-\frac{1}{2}}V(H_0+E)^{-k-\frac{1}{2}}$ lie in $\mathscr{I}_{2m/k}$ for $k = 1, 2, \ldots, m$. Thus picking E so that $\gamma < 1$ and expanding $|V|^{\frac{1}{2}}(H+E)^{-m}$, we get a sum over q and l of terms of the form

$$(|V|^{\frac{1}{2}}(H_0+E)^{-\ell_0-\frac{1}{2}})\left[\prod_{i=1}^{q}(H_0+E)^{-\frac{1}{2}}V(H_0+E)^{-\ell_i-\frac{1}{2}}\right](H_0+E)^{-\frac{1}{2}} \quad (60)$$

with $\sum_{i=0}^{q}\ell_i = m$. Using Hölder's inequality for trace ideals, this term is Hilbert-Schmidt with a norm bounded by $c\gamma^q$, so the sum of the Hilbert-Schmidt norms converges. ∎

This last result is somewhat disappointing in that it requires V to be in L^1, and thus it must have $|x|^{-n-\varepsilon}$ falloff more or less. On the other hand, we have existence so long as V has $|x|^{-1-\varepsilon}$ falloff. We shall later prove completeness under these conditions also but only by using more sophisticated methods; see Section XIII.8, Theorem XIII.33 or Section 17 of this chapter. It turns out that in case V is spherically symmetric, the Kato-Birman theory is applicable even if one has only $|x|^{-1-\varepsilon}$ falloff.

Theorem XI.31 Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and let $V(x) = V(|x|)$ be a function of $r = |x|$ alone. Suppose that

$$\int_1^\infty |V(r)|\,dr + \int_0^1 r|V(r)|\,dr < \infty \quad (61)$$

Then V is H_0-form bounded with relative bound zero and $\Omega^{\pm}(H, H_0)$ exist and are complete.

Proof Let us decompose $L^2(\mathbb{R}^3) = \oplus_{\ell=0}^{\infty}\oplus_{m=-\ell}^{\ell}\mathscr{h}_{\ell m}$ where $\mathscr{h}_{\ell m} = \{rf(r)Y_{\ell m}(\theta)\}$. Each $\mathscr{h}_{\ell m}$ is isomorphic to $L^2(0,\infty; dr) \equiv \mathscr{H}$ under the correspondence $rf(r)Y_{\ell m} \leftrightarrow f(r)$ (see Example 4 of the Appendix to Section X.1). Let $h_{0,\ell} = -(d^2/dr^2) + \ell(\ell+1)r^{-2}$ on $\mathscr{H}$ with boundary condition $f(0) = 0$ when $\ell = 0$. Let $h_0 = h_{0,0}$. Then H_0 is isomorphic to $\oplus_{\ell,m}h_{0,\ell}$. Let v be multiplication by V on $\mathscr{H}$. We shall prove that

$$\mathrm{Tr}(|v|^{\frac{1}{2}}(h_0+1)^{-1}|v|^{\frac{1}{2}}) < \infty \quad (62)$$

This implies that $\lim_{E\to\infty}\||v|^{\frac{1}{2}}(h_0+E)^{-1}|v|^{\frac{1}{2}}\| = 0$ so that $|v|$ is h_0 form bounded with relative bound zero. Since $h_0 \le h_{0,\ell}$, we obtain that V is H_0 form bounded with relative bound zero. Let $h_\ell = h_{0,\ell} + v$. Decompose

$$(h_\ell+E)^{-1} - (h_{0,\ell}+E)^{-1} = ABCD$$

where $A = (h_\ell+E)^{-1}(h_0+1)^{\frac{1}{2}}$ and $D = (h_0+1)^{\frac{1}{2}}(h_{0,\ell}+E)^{-1}$ are bounded and $B = (h_0+1)^{-\frac{1}{2}}|v|^{\frac{1}{2}}$ and $C = [v/|v|^{\frac{1}{2}}](h_0+1)^{-\frac{1}{2}}$ are Hilbert-Schmidt by (62). It follows, by the Kuroda-Birman theorem that $\Omega^{\pm}(h_\ell, h_{0,\ell})$ exist and are complete so that $\Omega^{\pm}(H, H_0)$ exist and are complete.

Thus, we need only prove that (62) holds. We claim that

$$\mathrm{Tr}(|v|^{\frac{1}{2}}(h_0+1)^{-1}|v|^{\frac{1}{2}}) = \int_0^\infty |V(r)|[e^{-r}(\sinh r)]\,dr \quad (63)$$

From this, (62) follows by using (61) and the estimates

$$\sinh r \le e^r, \qquad \sinh r \le r\cosh r \le re^r$$

for $r \ge 0$. Now, $(h_0+1)^{-1}$ is an integral operator with kernel

$$(h_0+1)^{-1}(r,r') = e^{-u}\sinh w \qquad u = \max\{r,r'\},\quad w = \min\{r,r'\}$$

as can be checked easily (Problem 47). Thus $|v|^{\frac{1}{2}}(h_0+1)^{-1}|v|^{\frac{1}{2}}$ has an integral kernel

$$K(r,r') = |v(r)|^{\frac{1}{2}}(h_0+1)^{-1}(r,r')|v(r')|^{\frac{1}{2}}$$

so (63) corresponds to the formula

$$\mathrm{Tr}(A) = \int_0^\infty K(r,r)\,dr \quad (64)$$

While (64) is heuristically just a continuum analogue of the fact that $\mathrm{Tr}(a_{ij}) = \sum_i a_{ii}$ for finite matrices, it is *not* a general fact for integral operators; this is obvious since $K(r,r')$ is determined only a.e. and $\{(r,r')|r=r'\}$ has measure zero! Nevertheless (64) does hold when the kernel $K(r,r')$ is continuous and the operator is positive semidefinite—we shall prove this as a lemma below. The lemma implies (63) when V is continuous, and a simple approximation argument (Problem 48) concludes the proof of (63) for general V. ∎

Lemma Let μ be a Baire measure on a locally compact Haudorff space X. Let $\mathscr{H} = L^2(X, d\mu)$ and let K be a continuous function on $X \times X$. Suppose that:

(i) For any $\varphi \in \kappa(X)$, the continuous functions of compact support, $\iint \overline{\varphi(x)}\varphi(y)K(x,y)\,d\mu(x)\,d\mu(y) \ge 0$. It follows that $K(x,x) \ge 0$.
(ii) $\int K(x,x)\,d\mu(x) < \infty$.

Then, there is a trace class operator A with integral kernel K. Moreover,

$$\mathrm{Tr}(A) = \int K(x,x)\,d\mu(x) \quad (65)$$

Conversely, if A is a positive trace class operator with a continuous kernel K, then (ii) holds and (65) is true.

Proof Suppose that (i) and (ii) hold. Let f be in $\kappa(X)$ and let $K_f(x, y) = f(x)K(x, y)f(y)$. Then K_f is in $L^2(X \times X, d\mu \otimes d\mu)$ so that there is a Hilbert-Schmidt operator A_f with kernel K_f. Let $\{U_1, \ldots, U_n\} = \mathcal{U}$ be a finite set of disjoint Baire sets of finite μ measure and let $P_{\mathcal{U}}$ be the projection in $\mathcal{H}$ onto the span of the characteristic functions of the U_i. Then

$$\operatorname{Tr}(P_{\mathcal{U}} A_f P_{\mathcal{U}}) = \sum_i \int_{U_i \times U_i} \mu(U_i)^{-1} f(x)K(x, y)f(y)\, d\mu(x)\, d\mu(y) \tag{66}$$

Order the $\mathcal{U}$'s by $\mathcal{U} < \mathcal{U}'$ if $\bigcup U_i \subset \bigcup U_i'$ and each U_i' is either disjoint from all the U_i' or contained in some U_i, that is, if and only if Ran $P_{\mathcal{U}} \subset$ Ran $P_{\mathcal{U}'}$. Under this ordering, the set of $\mathcal{U}$'s is a net and: (a) $P_{\mathcal{U}}$ is monotone increasing in $\mathcal{U}$: (b) s-lim $P_{\mathcal{U}} = 1$; (c) as $\mathcal{U}$ goes to "infinity," the right-hand side of (66) converges to $\int f(x)^2 K(x, x)\, d\mu(x)$. By (i), (a), and (b)

$$\operatorname{Tr}(A_f) = \lim_{\mathcal{U}} \operatorname{Tr}(P_{\mathcal{U}} A_f P_{\mathcal{U}})$$

(both sides may be infinite a priori) and so by (c) and (ii), A_f is trace class and

$$\operatorname{Tr}(A_f) = \int f(x)^2 K(x, x)\, d\mu(x)$$

Now order all f's with $0 \le f \le 1$ and $f \in \kappa(X)$ by pointwise inequality. Then, for any $\varphi \in \mathcal{H}$,

$$(\varphi, A_f \varphi) \le \|\varphi\|^2 \operatorname{Tr}(A_f) \le \|\varphi\|^2 \int K(x, x)\, d\mu(x)$$

Moreover, for $\varphi \in \kappa(X)$, $\lim_{f \nearrow 1} (\varphi, A_f \varphi)$ trivially exists. By a density argument, and polarization, w-$\lim_{f \nearrow 1} A_f = A$ exists. Moreover, for any finite rank operator B,

$$|\operatorname{Tr}(AB)| = \lim_{f \nearrow 1} |\operatorname{Tr}(A_f B)| \le \|B\| \lim_{f \nearrow 1} \operatorname{Tr}(A_f) \le \|B\| \int K(x, x)\, d\mu(x)$$

Thus A is trace class. Taking φ's in $\kappa(X)$, we find that $K(x, y)$ is the integral kernel for A. Finally, (65) follows by repeating the $P_{\mathcal{U}}$ argument.

The converse statement follows from the $P_{\mathcal{U}}$ argument also. ∎

Example 1 (scattering in a magnetic field) Let $H_0 = -\Delta$ on L^2 and

$$H = \sum (i\,\partial_j - a_j(x))^2 + V(x)$$

where V, a_j, a_j^2 are in $L^2_\delta(\mathbb{R}^n)$ with $\delta > \frac{1}{2}n$. Suppose moreover that $Q(H) = Q(H_0)$ so that $(H + E)^{-\frac{1}{2}}\, \partial_j$ are bounded. Then, for any bounded interval I, the four operators

$$E_I(H)\, \partial_j a_j E_I(H_0), \qquad E_I(H) a_j\, \partial_j E_I(H_0),$$
$$E_I(H) a_j^2 E_I(H_0), \qquad \text{and} \qquad E_I(H) V E_I(H_0)$$

are trace class. The last three are trace class by Theorem XI.21 even without the factor of $E_I(H)$. The first is trace class since $E_I(H)\, \partial_j$ is bounded and $a_j E_I(H_0)$ is trace class. It follows that $E_I(H)(H - H_0)E_I(H_0)$ is trace class so that, since $Q(H) = Q(H_0)$, Birman's theorem is applicable. We conclude that $\Omega^{\pm}(H, H_0)$ exist and are complete.

Example 2 This is a nonphysical example, but it shows the power of Birman's theorem. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$. Let a be in $L^2_\delta(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$ and grad a be in $L^2_\delta(\mathbb{R}^n)$, $\delta > \frac{1}{2}n$, and suppose $a \ge 0$. Define

$$H = H_0 + \Delta a \Delta$$

as a sum of quadratic forms. Since $\Delta a \Delta$ is a fourth-order operator, it is a very singular perturbation of H_0. Clearly $Q(H) = Q(H_0) \cap D(a^{\frac{1}{2}}\Delta) \subset Q(H_0)$. Moreover, $D(H_0) \subset Q(H)$. Thus H and H_0 are mutually subordinate. Writing $H - H_0 = \sum_j (\partial_j)a(\partial_j \Delta) + \partial_j(\partial_j a)\Delta$ and using the fact that $E_I(H)\, \partial_j$ is bounded as in Example 1, we see that

$$E_I(H)(H - H_0)E_I(H_0) \in \mathscr{I}_1$$

so that $\Omega^{\pm}(H, H_0)$ exist and are complete by Birman's theorem.

Theorem XI.25 asserts that local singularities of V are inessential to the question of existence of $\Omega^{\pm}(-\Delta + V, -\Delta)$. One can ask whether they are also irrelevant to completeness; to a large extent the answer is yes as we shall now describe.

Definition A self-adjoint operator H is called a **strongly semibounded local perturbation of $H_0 = -\Delta$** if and only if:

(i) $Q(H) \subset Q(H_0)$ and $H_0 \le c_1(H + c_2)$ for suitable constants c_1 and c_2.
(ii) If $f \in \mathscr{D}_{L^\infty}$, the C^∞ functions with $D^\alpha f \in L^\infty$ for all α, and $\varphi \in D(H)$, then $f\varphi \in D(H)$ and

$$H(f\varphi) = f(H\varphi) - 2\nabla f \cdot \nabla\varphi - \varphi\, \Delta f \tag{67}$$

Notice that, by (i), if φ is in $D(H)$, then $\nabla\varphi$ is in L^2. (ii) says that in some sense $H - H_0$ is a multiplication operator.

Proposition

(a) Let $V = V_1 + V_2$ where $V_1 \geq 0$ and in $L^1_{1\infty}$ and V_2 is $-\Delta$-form bounded with relative bound $\alpha < 1$. Then $H = -\Delta + V$ defined as a form sum on $Q(H_0) \cap Q(V_1)$ is a strongly semibounded local perturbation of H_0.

(b) Suppose that W also obeys the conditions of (a). Let $\tilde{H} = -\Delta + W$. If $f \in \mathscr{D}_{L^\infty}$ has support in $\{x \mid V(x) = W(x)\}$, then for all $\varphi \in D(H)$, we have $f\varphi \in D(\tilde{H})$ and $\tilde{H}(f\varphi) = H(f\varphi)$.

Proof (a) Condition (i) is easy, so we need only check condition (ii). Let $\varphi \in C_0^\infty$ and $f \in \mathscr{D}_{L^\infty}$. Then clearly $f\varphi \in Q(-\Delta)$ and

$$\nabla(f\varphi) = f\nabla\varphi + \varphi\,\nabla f$$

By an easy limiting argument, it follows that if $\varphi \in Q(-\Delta)$, then $f\varphi \in Q(-\Delta)$. Let $\varphi \in Q(-\Delta)$ and $\psi \in C_0^\infty$. Then

$$(\varphi, (-\Delta)f\psi) = (f\varphi, (-\Delta)\psi) - 2((\nabla f)\varphi, \nabla\psi) - ((\Delta f)\varphi, \psi)$$

Again, using a limiting argument, this extends to all $\psi \in Q(H_0)$. Clearly, if $\int V_1 |\varphi|^2\, dx < \infty$, we have that $\int V_1 |f|^2 |\varphi|^2\, dx < \infty$; so if $\psi, \varphi \in Q(H)$, then $f\varphi \in Q(H)$ and

$$(\psi, H(f\varphi)) = (f\psi, H\varphi) - 2((\nabla f)(\psi, \nabla\varphi) - ((\nabla f)\psi, \varphi) \tag{68}$$

Recall that by the form construction (Section VIII.6) the domain of H consists of those φ in $Q(H)$ such that there is an $\eta \in \mathscr{H}$ satisfying $(\psi, \eta) = (\psi, H\varphi)$ for all ψ in $Q(H)$. In this case $\eta = H\varphi$. Given this and (68), we conclude that if $\varphi \in D(H)$, then $f\varphi$ is in $D(H)$ and (67) holds.

(b) Since $\varphi \in D(H) \subset Q(H)$, $\varphi \in Q(H_0)$ and $\int |\varphi|^2 V_1\, dx < \infty$. Since $V = W$ on $\operatorname{supp} f$, $\int |f|^2 |\varphi|^2 W_1\, dx < \infty$ so $\varphi \in Q(\tilde{H})$. By (ii), $(\psi, H(f\varphi)) = (\psi, \tilde{H}(f\varphi))$ for all $\psi \in Q(H_0)$ so that $f\psi$, $(\nabla f)\psi$, $(-\Delta f)\psi \in Q(V_1)$. Since any $\psi \in Q(W_1)$ has this property, $H = \tilde{H}$. ∎

Theorem XI.32 Let H be a strongly semibounded local perturbation of $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$. Let W be a function obeying:

(i) W is H_0-form bounded with relative bound $\alpha < 1$. Let $\tilde{H} = -\Delta + W$ be defined as a form sum.

(ii) $H = -\Delta + W$ outside the sphere of radius R, in the sense that if $f \in \mathscr{D}_{L^\infty}$ has support in $\{x \mid |x| > R\}$, and $\varphi \in D(H)$ or $\varphi \in D(\tilde{H})$, then $f\varphi \in D(H) \cap D(\tilde{H})$ and $H(f\varphi) = \tilde{H}(f\varphi)$.

(iii) $\Omega^\pm(\tilde{H}, H_0)$ exist and are complete.

Then $\Omega^\pm(H, H_0)$ exist and are complete.

Proof By the chain rule and Proposition 3 of Section 3, it suffices to prove that $\Omega^\pm(H, \tilde{H})$ and $\Omega^\pm(\tilde{H}, H)$ exist. Let J be multiplication by a function in $\mathscr{D}_{L^\infty}$ that vanishes if $|x| < R$ and is 1 if $|x| > 2R$. Since $Q(H) \subset Q(H_0)$ and $Q(\tilde{H}) \subset Q(H_0)$, $(H + c)^{-1/2}(H_0 + 1)^{1/2}$ and $(\tilde{H} + c)^{-1/2}(H_0 + 1)^{1/2}$ are bounded for c sufficiently large. Thus $(1 - J)(H + c)^{-1/2}$ and $(1 - J) \times (\tilde{H} + c)^{-1/2}$ are in $\mathscr{I}_p$ if $p > \max\{n, 2\}$ by Theorem XI.20, and in particular are compact. Therefore $\Omega^\pm(H, \tilde{H}; 1 - J)$ and $\Omega^\pm(\tilde{H}, H; 1 - J)$ exist (and are in fact zero) by Lemma 2 of Section 3 and Problem 18. We are thus reduced to showing that $\Omega^\pm(H, \tilde{H}; J)$ and $\Omega^\pm(\tilde{H}, H; J)$ exist.

We claim that by mimicking the proof of Birman's theorem, it suffices to prove that, for any bounded interval I,

$$E_I(H)(HJ - J\tilde{H})E_I(\tilde{H}) \in \mathscr{I}_1 \tag{69}$$

For by hypothesis (ii), $JD(H) \subset D(\tilde{H})$, $JD(\tilde{H}) \subset D(H)$, so that the necessary subordinate condition holds: $(\tilde{H} + c)^{-1}J(H + c)$ and $(H + c)^{-1}J(\tilde{H} + c)$ are bounded. By (67) and hypothesis (ii), $(HJ - J\tilde{H})\varphi = -2\nabla \cdot (\nabla J)\varphi - (\Delta J)\varphi$ for $\varphi \in D(\tilde{H})$. Since $Q(H_0) \supset Q(H) \supset \operatorname{Ran} E_I(H)$, we have that $(E_I(H))\nabla$ is bounded. Thus, because ∇J, $\Delta J \in C_0^\infty$ and $(\tilde{H} + c)^\ell E_I(\tilde{H})$ is bounded, we need only prove that for some integer ℓ and any $g \in C_0^\infty$,

$$g(\tilde{H} + c)^{-\ell} \in \mathscr{I}_1 \tag{70}$$

By hypothesis (i), $(H_0 + c)^{\frac{1}{2}}(\tilde{H} + c)^{-\frac{1}{2}}$ is bounded. By Theorem XI.22,

$$g(H_0 + c)^{-\frac{1}{2}} \in \mathscr{I}_q \tag{71}$$

so long as $q > n$. Thus

$$g(\tilde{H} + c)^{-\frac{1}{2}} \in \mathscr{I}_q \tag{72}$$

for $q > n$. Let $A = (\tilde{H} + c)$ and $D = \partial_i$. We first claim that

$$gA^{-1} \quad \text{and} \quad DgA^{-1} \quad \text{are in } \mathscr{I}_q \tag{73}$$

The first statement is obvious from (72) and the second follows from the boundedness of $DA^{-\frac{1}{2}}$, (72), and the calculation:

$$\begin{aligned} DgA^{-1} &= DA^{-1}g + D[A^{-1}, g] \\ &= DA^{-1}g + DA^{-1}DhA^{-1} + DA^{-1}fA^{-1} \end{aligned}$$

where $h = 2\nabla \cdot g, f = -\Delta g \in C_0^\infty$. A calculation similar to this shows that

$$\begin{aligned} gA^{-j-1} &= A^{-1}gA^{-j} + [g, A^{-1}]A^{-j} \\ &= A^{-1}gA^{-j} - A^{-1}DhA^{-j-1} - A^{-1}fA^{-j-1} \end{aligned} \tag{74}$$

It follows from (73), (74) that if $gA^{-j} \in \mathscr{I}_r$ for all $g \in C_0^\infty$, then $gA^{-j-1} \in \mathscr{I}_s$ for all $g \in C_0^\infty$ where $s^{-1} = \min\{1, r^{-1} + q^{-1}\}$. Thus starting with (73), we see inductively that for all $g \in C_0^\infty$, $gA^{-j} \in \mathscr{I}_{q_j}$ where $q_j = \min\{1, jq^{-1}\}$. Taking $\ell > q$, (70) holds. ∎

Corollary If $V = V_1 + V_2$ has compact support where $V_1 \geq 0$, $V_1 \in L^1$ and V_2 is $-\Delta$-form bounded with relative bound $\alpha < 1$, then $\Omega^\pm(-\Delta + V, -\Delta)$ exist and are complete.

The condition that $H_0 \leq c_1(H + c_2)$ is critical for the above results as the following spectacular example shows.

Thus far in this section we have presented a way of proving Ran $\Omega^+ =$ Ran Ω^- that works in particular for $-\Delta + V$ with $V \in C_0^\infty(\mathbb{R}^3)$. We shall later discuss other methods of proving asymptotic completeness. Lest the reader think that asymptotic completeness must hold, we mention the existence of certain pathological examples:

Counterexample There exists a potential V that is bounded on compact subsets $\mathbb{R}^3\backslash\{0\}$ so that:

(i) V has compact support in $\mathbb{R}^3$.
(ii) $H = -\Delta + V$ is essentially self-adjoint on $D(-\Delta) \cap D(V)$.
(iii) $-\Delta + V$ is a positive operator.
(iv) The wave operators $\Omega^\pm = \text{s-lim}_{t \to \mp\infty} e^{itH}e^{-itH_0}$ exist.

but

(v) Ran $\Omega^+ \neq$ Ran Ω^-.

Let us describe the potential V which has been constructed by D. Pearson. There are basic building blocks of size $8(a + a^4)$ consisting of eight square wells as shown in Figure XI.3. Now define a_n by $8(a_n + a_n^4) = 2^{-n}$. The potential V will be a function W of $|\mathbf{r}|$. W will be 0 on $(1, \infty)$, and equal to the basic block potential with $a = a_{n+1}$ on $(2^{-n-1}, 2^{-n})$. Thus V is schema-

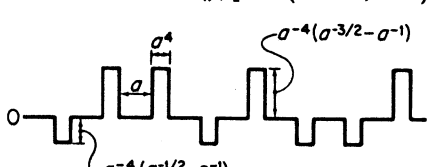


FIGURE XI.3 Pearson's building blocks.

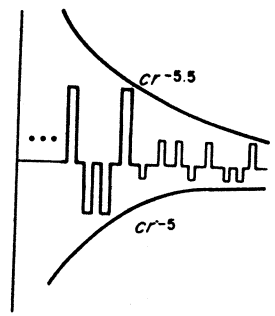


FIGURE XI.4 Schematic of Pearson's potential.

tically shown in Figure XI.4: It does not get larger than $cr^{-5.5}$ or smaller than $-cr^{-5}$, and its maximum oscillations approximately reach these curves. Notice also that it is "mostly" zero as $r \to 0$.

Physically, the reason for the breakdown of asymptotic completeness is that there exist incoming waves which in the future have two pieces, one of which scatters outward and another which gets trapped near the origin. Because of the positive bumps, the particle is prevented from reaching the origin in finite time, which is why H is essentially self-adjoint. The negative bumps prevent the particle from just bouncing off. We shall not prove the claimed properties for V, but refer the reader to the reference in the Notes.

To illustrate the wide applicability of the methods we have described, we consider two last examples, one a model of scattering from a thin slab of matter and the other of scattering from a semi-infinite chunk of matter.

Example 3 Let W be a function on $\mathbb{R}^3$ obeying

$$|W(x)| \leq C_1(1 + |x|)^{-\alpha}$$

Fix k and let

$$V(x) = \sum_{\substack{n_1 = 0, \ldots, k \\ n_2, n_3 \in \mathbb{Z}}} W(x_1 - n_1, x_2 - n_2, x_3 - n_3)$$

So long as $\alpha > 2$, the method of estimating sums by integrals easily shows that the sum converges and

$$|V(x)| \leq C(1 + |x_1|)^{-(\alpha-2)}$$

The wave operators $\Omega^\pm(-\Delta + V, -\Delta)$ describe the scattering of a single particle from an array of particles in a slab of $k + 1$ planes of scattering sites. If $\hat{u}$ is C^∞ with compact support away from points where $k_1 = 0$, it is easy to see that

$$\|Ve^{+it\Delta}u\|_2 \leq (1 + |t|)^{-(\alpha-2)}$$

by using stationary phase methods. It follows that, if $\alpha > 3$, $\Omega^{\pm}(-\Delta + V, -\Delta)$ will exist. Moreover, one can prove that Ran Ω^{+} = Ran Ω^{-} as follows: The function V is periodic in the 2 and 3 directions; and for that reason, $H = -\Delta + V$ has a (direct integral) decomposition as a fibered operator in the sense of Section XIII.16. The situation is somewhat different than that in Section XIII.16, where we discuss potentials periodic in all three directions. In that case the fibers are operators with purely discrete spectrum. In this case the fibers $H_0(k)$ for $-\Delta$ have purely absolutely continuous spectrum, and the fibers $H(k)$ have some absolutely continuous spectrum but also the possibility of some eigenvalues. One shows that $(H(k) + i)^{-1} - (H_0(k) + i)^{-1}$ is trace class for all k from which it follows that Ran $\Omega^{+}(H, H_0)$ = Ran $\Omega^{-}(H, H_0) = \int^{\oplus} P_{ac}(H(k))\, dk$. For details in the above construction, the reader should consult the reference in the Notes. We remark that it may happen that the $H(k)$ have point spectrum contributing to absolutely continuous spectrum of H (as in Section XIII.16) in which case Ran Ω^{+} = Ran $\Omega^{-} \neq$ Ran $P_{ac}(H)$.

Example 4 Let W be a bounded periodic function on $\mathbb{R}$ and let $H_0 = -d^2/d^2x$, $H_1 = H_0 + W$. As we shall describe in Section XIII.16, H_1 is a model for the motion of an electron in a solid. Let

$$V(x) = \begin{cases} W(x), & x > 0 \\ 0, & x \leq 0 \end{cases}$$

so that $H = H_0 + V$ describes a model for electron scattering off a large (idealized as semi-infinite) chunk of solid. One expects that as $t \to \infty$ any solution $e^{-iHt}\varphi$ with $\varphi \in$ Ran $P_{ac}(H)$ should approach a sum of a free plane wave moving to the left and a solution $e^{-iH_1 t}\psi$ moving to the right in the solid. Let us prove this.

Let J be multiplication by a C^{∞} function φ on $\mathbb{R}$ that is 0 on $(-\infty, -1)$ and 1 on $(1, \infty)$. Then, as in the proof of Theorem XI.32, $E_l(A) \times (AJ - JB)E_l(B)$ is trace class for any of the five possibilities obtained as $\langle A, B\rangle$ run through $\langle H_0, H_0\rangle, \langle H_1, H_1\rangle, \langle H, H\rangle, \langle H, H_1\rangle, \langle H_1, H\rangle$, and the same is true if J is replaced by $1 - J$ and H_0 and H_1 are interchanged. Moreover, since $D(H_1) = D(H) = D(H_0)$ and $JD(H_0) \subset D(H_0)$, all pairs are mutually subordinate.

Now, for $B = H, H_1, H_0$, define

$$P_r^{\pm}(B) = \Omega^{\pm}(B, B; J), \qquad P_\ell^{\pm}(B) = \Omega^{\pm}(B, B; 1 - J)$$

where the limits exist by the above and Birman's theorem. Since $J^* = J$ and

$(J^2 - J)(B + 1)^{-1}$ is compact, the $P_{\ell,r}^{\pm}(B)$ are all orthogonal projections with

$$P_\ell^{\pm}(B) + P_r^{\pm}(B) = P_{ac}(B) \qquad \text{and} \qquad P_\ell^{\pm}(B)P_r^{\pm}(B) = 0$$

by the intertwining relations for $\Omega^{\pm}(A, B; J)$. Moreover, Ran $P_\ell^{\pm}(B)$ is precisely the set of $\varphi \in$ Ran $P_{ac}(B)$ so that $e^{-itB}\varphi$ moves off to $-\infty$ as $t \to \mp\infty$ in the sense that

$$\lim_{t \to \mp\infty} \int_a^{\infty} |(e^{-itB}\varphi)(x)|^2\, dx = 0$$

for any a.

Let

$$W_0^{\pm} = \Omega^{\pm}(H, H_0; 1 - J), \qquad W_1^{\pm} = \Omega^{\pm}(H, H; J)$$

Using the above results, it is not hard to show that these operators exist and that $W_0^{\pm}$ are a partial isometries with initial spaces $P_\ell^{\pm}(H_0)$ and final spaces $P_\ell^{\pm}(H)$. The same is true if W_0 is replaced by W_1, H_0 by H_1 and ℓ by r. Thus $P_{ac}(H) = P_\ell^{\pm}(H) + P_r^{\pm}(H)$ implies that $P_{ac}(H) =$ Ran $W_0^{\pm} \oplus$ Ran $W_1^{\pm}$, which is the desired completeness statement.

An interesting consequence of the above is that if ψ is a vector with the support of $\hat{\psi}$ in (a, b) where $a > 0$ and (a^2, b^2) is inside a gap for H_1 (we shall show in Section XIII.16 that H_1 has spectrum $\bigcup_i [\alpha_i, \beta_i]$ with $\alpha_1 < \beta_1 \leq \alpha_2 < \beta_2 \leq \cdots$ where "typically" the "gaps" (β_i, α_{i+1}) are nonempty), then $W_0^{-}\psi \in$ Ran W_0^{+}; that is, a particle sent in at an energy in the gap is totally reflected. One can combine the above ideas with those in Example 3 and treat scattering from a half-space of higher dimensional crystal, or scattering from various kinds of crystal defects. These subjects and the details of the above construction are treated in the reference in the Notes.

We conclude this section with a formal definition and discussion of the scattering operator in two-body quantum mechanics. In interpreting experimental scattering data, the natural question is the following: We prepare a state that in the past looks like the state $e^{-iH_0 t}\varphi$, and we want to know how it looks in the future, that is, we look at $e^{-iHt}\Omega^{+}\varphi$. We ask: What is the probability of finding that this state is the free state $e^{-iH_0 t}\psi$ asymptotically in the future? By the rules of quantum mechanics, this probability $P_{\varphi \to \psi}$ is given by

$$\begin{aligned} P_{\varphi \to \psi} &= |(\Omega^{-}\psi, \Omega^{+}\varphi)|^2 \\ &= |(\psi, (\Omega^{-})^*\Omega^{+}\varphi)|^2 \end{aligned}$$

Definition If $\Omega^{\pm}$ exist, we define the ***S*-matrix, *S*-operator**, or scattering operator by

$$S = (\Omega^{-})^*\Omega^{+}$$

Notice that this definition makes sense even if Ran Ω^+ does not equal Ran Ω^-. While completeness is not needed to define S, it is equivalent to S being unitary.

We shall discuss S in detail in Sections 6 and 8. At this point, we note some simple properties of S (Problem 49).

Proposition

(a) $Se^{iH_0t} = e^{iH_0t}S$ for all t. S leaves $D(H_0)$ invariant; and if $\psi \in D(H_0)$, then $H_0(S\psi) = S(H_0\psi)$.
(b) If U is any unitary operator that commutes with H and H_0, then $US = SU$. In particular, if V is rotationally invariant, then S is rotationally invariant.
(c) $\overline{(S\psi)}(x) = (S^*\bar{\psi})(x)$.
(d) S is unitary if and only if Ran $\Omega^+ =$ Ran Ω^-.

(c) is called time reversal invariance for reasons discussed in the Notes.

On account of the continuity properties proved for the correspondence $A, B \mapsto \Omega^{\pm}(A, B)$ within the Kato–Birman theory, S has continuity properties. Typical is the following:

Proposition Let V_n and V_∞ be in $L^{3/2}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ and suppose that $\lim_{n\to\infty} \|V_n - V_\infty\|_1 = 0$ and $\sup_n \|V_n\|_{3/2} < \infty$. Let $S(V)$ be the S-matrix for $-\Delta + V$. Then

$$\text{s-lim}_{n\to\infty} S(V_n) = S(V_\infty)$$

Proof By mimicking the proof of Theorem XI.30, one sees (Problem 50) that $(H_n + i)^{-1} \to (H_\infty + i)^{-1}$ in trace class norm. Thus, by Problem 28,

$$\Omega^{\pm}(H_n, H_0) \to \Omega^{\pm}_\infty$$

strongly, so $S_n \to S$ weakly. But by completeness, the S_n and S are all unitary, so $S_n \to S$ strongly. ∎

There is one final property of $\Omega^{\pm}$ and S which we would like to discuss. We defer the full physical interpretation of this result until we prove a similar result for N-body systems, but we note that if we have scattering from a fixed scattering center and we take a fixed state and translate it toward infinity, it will miss the scattering center (see Figure XI.5).

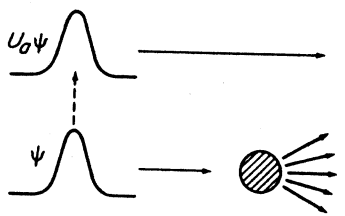


FIGURE XI.5 The cluster property.

Theorem XI.33 Under the hypotheses of Theorem XI.24

$$\text{s-lim}_{a\to\infty} U_a^{-1}\Omega^{\pm}U_a = I$$

$$\text{s-lim}_{a\to\infty} U_a^{-1}SU_a = I$$

where U_a are the operators $(U_a f)(\mathbf{r}) = f(\mathbf{r} - \mathbf{a})$.

Proof We shall prove that s-$\lim_{a\to+\infty} U_a^{-1}\Omega^{\pm}U_a = I$, from which it follows that w-$\lim_{a\to\infty} U_a^{-1}SU_a = I$. Since $\|U_aSU_a^{-1}\| \le 1$, this implies that s-$\lim_{a\to\infty} U_a^{-1}SU_a = I$.

By an $\varepsilon/3$ argument, we need only prove that

$$\lim_{a\to\infty} (U_a^{-1}(\Omega^{\pm} - 1)U_a)\varphi = 0$$

for all $\varphi \in \mathscr{S}$. For such φ,

$$U_a^{-1}(\Omega^{\pm} - 1)U_a\varphi = \mp i\int_0^{\mp\infty} (U_a^{-1}e^{iHt}Ve^{-iH_0t}U_a)\varphi\, dt$$

Let $F_a(t)$ denote $\|U_a^{-1}e^{-iHt}Ve^{-iH_0t}U_a\varphi\|$. It is easy to check that $F_a(t) = \|V_a e^{-iH_0t}\varphi\|$ where $V_a(r) = V(r + a)$. Looking at the second proof of Theorem XI.24, we see that $F_a(t)$ is bounded by an L^1 function of t uniformly in a because the L^p-norm of V_a is independent of a. By the dominated convergence theorem, it thus suffices to show that $F_a(t) \to 0$ for each fixed t. Since e^{-iH_0t} leaves $\mathscr{S}$ invariant, we need just show that $\lim_{a\to\infty} \|V_a\varphi\| = 0$ for all $\varphi \in \mathscr{S}$ and this is easy. ∎

XI.5 Quantum scattering II: N-body case

Scattering theory for N-body quantum systems is complicated for two reasons, one kinematical and one dynamical. The kinematic reason appears already for $N = 3$. Before one removes the center of mass one has a natural

coordinate system $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$ in $\mathbb{R}^{3N} = \mathbb{R}^9$. Once we decide to take $\mathbf{R} = (\mu_1 + \mu_2 + \mu_3)^{-1}(\mu_1\mathbf{r}_1 + \mu_2\mathbf{r}_2 + \mu_3\mathbf{r}_3)$ as a variable, there is no natural choice for the other six coordinates. For example, we have the pairs $\langle \mathbf{r}_{12}, \mathbf{r}_{13}\rangle$ or $\langle \mathbf{r}_{12}, \mathbf{r}_{23}\rangle$ or $\langle \mathbf{r}_{13}, \mathbf{r}_{23}\rangle$ where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. Also, one might first change coordinates in the 1, 2 system to $\mathbf{R}_{12} = (\mu_1 + \mu_2)^{-1} \times (\mu_1\mathbf{r}_1 + \mu_2\mathbf{r}_2)$ and $\mathbf{r}_{12}$ and then go to the three-body system taking coordinates $\mathbf{R}$, $\mathbf{r}_{12}$, and $\zeta_2 = \mathbf{R}_{12} - \mathbf{r}_3$ (see Figure XI.6). The point is that various

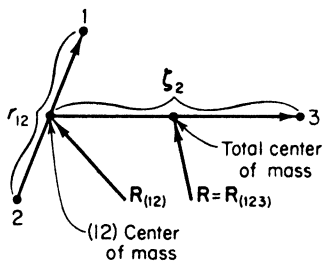


FIGURE XI.6 Jacobi coordinates, $N = 3$.

coordinates enter at various stages of the theory, and it is common to change coordinates in the middle of a proof. This kinematical complication is a nuisance.

The dynamical complication involves the richness of different sorts of scattering phenomena possible even for a three-body system. Suppose that particles 1 and 2 can form a bound state. Then one not only expects scattering of the "free" particles 1, 2, 3 into free particles (elastic three-body scattering) but also **capture processes** where "free" particles 1, 2, 3 are sent in and a bound state of 1 and 2 together with a "free" particle 3 comes out. These processes are indicated schematically in Figure XI.7a and b. Similarly, one

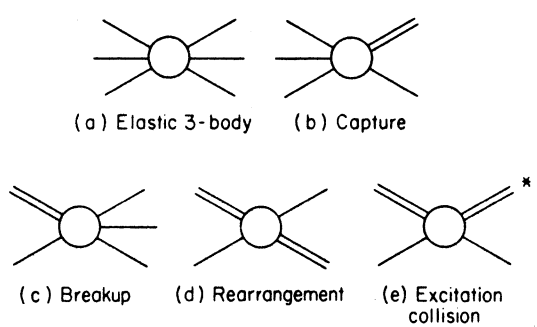


FIGURE XI.7 Three-body collision processes.

would like to describe **breakup processes** $(12) + 3 \to 1 + 2 + 3$ and **rearrangement collisions** $(12) + 3 \to 1 + (23)$ where (ij) represents a bound cluster of particles i and j. If there is more than one bound state of 1, 2, say (12) and (12)*, one can have **excitation collisions** $(12) + 3 \to (12)^* + 3$.

In the three-body case, we shall first enumerate the bound states of (12), (23), and (13) and for each such bound state b consider a "scattering channel." Instead of describing states that are asymptotically a three-free-particles state, we consider states that asymptotically consist of 1 and 2 bound in state b and 3 moving freely relative to (12). In the N-body case, we need to consider clustering into disjoint subsets $C_1, \ldots, C_k$ and a scattering channel for each k-tuple of bound states of $C_1, \ldots, C_k$. One expects scattering between channels. This complication is subtle and beautiful.

We begin by describing various coordinate systems. Consider the Hamiltonians

$$\tilde{H} = -\sum_{i=1}^{N}(2\mu_i)^{-1}\Delta_i + \sum_{i<j} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

$$\tilde{H}_0 = -\sum_{i=1}^{N}(2\mu_i)^{-1}\Delta_i$$

on $L^2(\mathbb{R}^{3N})$ where we write $\mathbf{r} = \langle \mathbf{r}_1, \ldots, \mathbf{r}_N\rangle \in \mathbb{R}^{3N}$ and $-\Delta_i$ is the Laplacian in the $\mathbf{r}_i$ variables. We now change coordinates to $\mathbf{R} = (\sum_{i=1}^N \mu_i)^{-1} \times \sum_{i=1}^N \mu_i\mathbf{r}_i$ and $N - 1$ additional 3-vector coordinates $\xi_1, \ldots, \xi_{N-1}$. These coordinates are required to satisfy two additional conditions: First, for each $i \neq j$, $\mathbf{r}_i - \mathbf{r}_j$ is required to be a linear combination of the ξ_i. Secondly, the differential operator $\tilde{H}_0$, when written in the new coordinates, is required to have no terms of the form $\nabla_{\mathbf{R}} \cdot \nabla_{\xi_i}$. Actually, as we shall see, the first condition implies the second. Such a coordinate system defines a decomposition $L^2(\mathbb{R}^{3N}) = L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^{3N-3})$ and a tensor decomposition of H and H_0:

$$\tilde{H} = h_0 \otimes 1 + 1 \otimes H$$

$$\tilde{H}_0 = h_0 \otimes 1 + 1 \otimes H_0$$

where $h_0 = -(2\sum_{i=1}^N \mu_i)^{-1}\Delta_{\mathbf{R}}$. The exact form of H depends on the coordinate system used for $\xi_1, \ldots, \xi_{N-1}$. As in the two-body case, one can think of a change of coordinates as an alternative description of the same operator or in terms of a unitary transformation. We shall take the former view. For some coordinate changes, the Jacobian will be a nonzero constant different from one, and it must thus be included in the inner product.

We consider three specific kinds of coordinate changes:

Atomic coordinates Let $\eta_i = \mathbf{r}_i - \mathbf{r}_N$. Then

$$H_0 = -\sum_{i=1}^{N-1} (2m_{iN})^{-1}\Delta_i + \sum_{i<j} (\mu_N)^{-1}\nabla_i \cdot \nabla_j$$

where $(m_{iN})^{-1} = \mu_i^{-1} + \mu_N^{-1}$, $\Delta_i = \Delta_{\eta_i}$, and $\nabla_i = \nabla_{\eta_i}$. Moreover,

$$H = H_0 + \sum_{i=1}^{N-1} V_{iN}(\eta_i) + \sum_{i<j<N} V_{ij}(\eta_i - \eta_j)$$

The reader is asked to carry through these computations in Problems 52a. As the name suggests, this coordinate system is especially useful in systems where one particle is distinguished from the others, such as atomic systems where the nucleus is distinguished. The additional terms $\sum_{i<j} \mu_N^{-1}\nabla_i \cdot \nabla_j$ are often a nuisance. They are called **Hughes–Eckart terms**. Notice that there are no cross terms in $\tilde{H}_0$ between $\mathbf{R}$ and η_i: It follows that for any choice of the ξ_i satisfying the first requirement above, the second requirement will automatically hold.

Jacobi coordinates Let

$$\zeta_i = \mathbf{r}_{i+1} - \left(\sum_{j\le i} \mu_j\right)^{-1}\left(\sum_{j\le i} \mu_j \mathbf{r}_j\right), \qquad i = 1, \ldots, N-1$$

Then (Problem 52b)

$$H_0 = -\sum_{i=1}^{N-1} (2\nu_i)^{-1}\Delta_{\zeta_i}$$

where $\nu_i^{-1} = \mu_{i+1}^{-1} + (\sum_{j\le i} \mu_j)^{-1}$ and $H = H_0 + \sum_{i<j} V_{ij}(\mathbf{r}_{ij})$ where $\mathbf{r}_{ij}$ is shorthand for $\mathbf{r}_i - \mathbf{r}_j$ written in terms of the ζ_j; for example,

$$\mathbf{r}_{41} = \zeta_3 + \frac{\mu_3}{\mu_1+\mu_2+\mu_3}\zeta_2 + \frac{\mu_2}{\mu_1+\mu_2}\zeta_1$$

Jacobi coordinates are obtained by first changing variables from $\langle \mathbf{r}_1, \mathbf{r}_2 \rangle$ to $\zeta_1 = \mathbf{r}_2 - \mathbf{r}_1$ and $\mathbf{R}_{(12)} = (\mu_1+\mu_2)^{-1}(\mu_1\mathbf{r}_1 + \mu_2\mathbf{r}_2)$, then from $\langle \mathbf{R}_{(12)}, \mathbf{r}_3 \rangle$ to $\zeta_2 = \mathbf{r}_3 - \mathbf{R}_{(12)}$, and $\mathbf{R}_{(123)} = (\mu_1+\mu_2+\mu_3)^{-1}[(\mu_1+\mu_2)\mathbf{R}_{(12)} + \mu_3\mathbf{r}_3]$, and so forth (see Figure XI.6). At each stage, one pair of variables is changed to a two-body center of mass and a relative coordinate. Since there are no cross terms in the change to center of mass coordinates for two-body systems, there are no Hughes–Eckart terms in the N-body H_0 above, which is the virtue of Jacobi coordinates. The disadvantage of Jacobi coordinates is the complicated form of $\mathbf{r}_{ij}$, although $\mathbf{r}_{12} = -\zeta_1$ is simple. Given any permutation $\langle i_1, \ldots, i_N \rangle$ of $\langle 1, \ldots, N \rangle$, there is an associated Jacobi coordinate system in which $\mathbf{r}_{i_1 i_2}$ is simple.

Clustered Jacobi coordinates The last coordinate system we discuss is particularly useful for scattering theory. In order to describe the breakup of an N-body system into bound clusters, we introduce some formal definitions and notation which will play an important role in this section and Section XIII.5.

Definition A partition D of $\{1, \ldots, N\}$ into k disjoint subsets $C_1, \ldots, C_k$ whose union is $\{1, \ldots, N\}$ is called a **cluster decomposition**. If $D = \{C_1, \ldots, C_k\}$ is a cluster decomposition and i, j are two numbers in $\{1, \ldots, N\}$, we write iDj if and only if i and j are in the same cluster C_ℓ and $\sim iDj$ if they are in different clusters. The symbols $\sum_{iDj}$ and $\sum_{\sim iDj}$ represent the sum over those pairs $\langle i, j \rangle$ with $i < j$ obeying iDj or $\sim iDj$, respectively.

Definition Let $D = \{C_\ell\}_{\ell=1}^k$ be a cluster decomposition. Let

$$\tilde{H}(C_\ell) = -\sum_{i\in C_\ell} (2\mu_i)^{-1}\Delta_i + \sum_{i<j,\, i,\, j\in C_\ell} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

and define $H(C_\ell)$, the **cluster Hamiltonian**, to be $\tilde{H}(C_\ell)$ with its center of mass removed.

$H(C_\ell)$ is an operator in $L^2(\mathbb{R}^{3N-3})$; it is independent of coordinates in the other clusters so $H(C_\ell) = h_{C_\ell} \otimes 1$ if we decompose $L^2(\mathbb{R}^{3N-3})$ as $L^2(\mathbb{R}^{3n_\ell-3}) \otimes L^2(\mathbb{R}^{3N-3n_\ell})$ where n_ℓ is the number of elements in C_ℓ. We shall henceforth use the symbol $H(C_\ell)$ for both the operator on $L^2(\mathbb{R}^{3N-3})$ and the operator on $L^2(\mathbb{R}^{3n_\ell-3})$ which we denoted above as h_{C_ℓ}. When we wish to emphasize which operator is intended, we shall talk about "$H(C_\ell)$ as an operator on $\mathscr{H}$" or "$H(C_\ell)$ as an operator on $\mathscr{H}_{C_\ell}$" where $\mathscr{H}_{C_\ell}$ is the space $L^2(\mathbb{R}^{3n_\ell-3})$ of functions of the internal coordinates of the cluster C_ℓ.

Definition Let $D = \{C_\ell\}_{\ell=1}^k$ be a cluster decomposition. The **intercluster potential** I_D is defined by

$$I_D = \sum_{\sim iDj} V_{ij}$$

Thus I_D is the sum of interactions between particles in different clusters.

Definition Let $D = \{C_\ell\}_{\ell=1}^k$ be a cluster decomposition. Let $\tilde{H}_D = \tilde{H} - I_D = \sum_{\ell=1}^k \tilde{H}(C_\ell)$ and define the **cluster decomposition Hamiltonian** H_D as the Hamiltonian $\tilde{H}_D$ with its center of mass removed. Thus

$$H_D = H - I_D$$

Since I_D depends only on coordinate differences $r_i - r_j$, it is unaffected by removal of the center of mass.

Notice that $H_D \neq \sum_{\ell=1}^{k} H(C_\ell)$; rather $H_D = T_D + \sum_{\ell=1}^{k} H(C_\ell)$ where T_D is the kinetic energy of the center of masses of the individual clusters with the total center of mass energy removed. Thus corresponding to the partition of the $3N-3$ coordinates in the k sets of internal coordinates for $C_1, \ldots, C_k$ plus the set of $3(k-1)$ coordinates describing the relative positions of the centers of mass of the clusters $\{C_i\}_{i=1}^{k}$, the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^{3N-3})$ is written as

$$\mathscr{H} = \mathscr{H}_D \otimes \mathscr{H}_{C_1} \otimes \mathscr{H}_{C_2} \otimes \cdots \otimes \mathscr{H}_{C_\ell}$$

and

$$\begin{aligned} T_D &= t_D \otimes 1 \otimes \cdots \otimes 1 \\ H(C_1) &= 1 \otimes h_{C_1} \otimes 1 \otimes \cdots \otimes 1 \\ &\vdots \\ H(C_\ell) &= 1 \otimes 1 \otimes \cdots \otimes h_{C_\ell} \end{aligned}$$

Clustered Jacobi coordinates are chosen precisely to make T_D simple. To obtain these coordinates we first change from $\langle \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle$ to

$$\langle \mathbf{R}_1, \ldots, \mathbf{R}_k, \xi_1^{(C_1)}, \ldots, \xi_{n_1-1}^{(C_1)}, \ldots, \xi_{n_k-1}^{(C_k)} \rangle$$

where

$$\mathbf{R}_\ell = \left(\sum_{i \in C_\ell} \mu_i \right)^{-1} \sum_{i \in C_\ell} \mu_i \mathbf{r}_i$$

and $\xi_1^{(C_\ell)}, \ldots, \xi_{n_\ell-1}^{(C_\ell)}$ are coordinates which together with the $\mathbf{R}_\ell$ form a set of coordinates for C_ℓ. For example, we could fix some $j \in C_\ell$ and let $\{\xi_m^{(C_\ell)}\}_{m=1}^{n_\ell-1} = \{\mathbf{r}_i - \mathbf{r}_j\}_{i \in C_\ell, i \neq j}$. Thus $H(C_\ell)$ is a differential operator in the variables $\xi_m^{(C_\ell)}$. Therefore

$$\tilde{H} = \sum_{\ell=1}^{k} (-2m_{C_\ell})^{-1} \Delta_{R_\ell} + \sum_{\ell=1}^{k} H(C_\ell) + I_D$$

where $m_{C_\ell} = \sum_{i \in C_\ell} \mu_i$. Now treat $\mathbf{R}_1, \ldots, \mathbf{R}_\ell$ as a set of k-body variables and take Jacobi coordinates $\{\zeta_\ell\}_{\ell=1}^{k-1}$ for $\langle \mathbf{R}_1, \ldots, \mathbf{R}_k \rangle$ as the first $k-1$ coordinates of a new coordinate system; $\{\xi_m^{(C_\ell)}\}$, where $1 \leq m \leq n_\ell - 1$ and $1 \leq \ell \leq k$, as the next $N-k$ coordinates and then the center of mass as the last coordinate. Then

$$H_D = \sum_{\ell=1}^{k-1} (-2M_\ell)^{-1} \Delta_{\zeta_\ell} + \sum_{\ell=1}^{k} H(C_\ell)$$

where $M_\ell^{-1} = m_{C_{\ell+1}}^{-1} + (\sum_{h \leq \ell} m_{C_h})^{-1}$. Thus we have a coordinate system in which H_D has a very simple form. The individual terms in the two sums depend on independent coordinates and thus commute with one another. Notice also that if $i \in C_1$, $j \in C_2$, then $\mathbf{r}_i - \mathbf{r}_j = -\zeta_1 + \xi_i^{(C_1)} - \xi_j^{(C_2)}$ where $\xi_i^{(C_\ell)}$ is some combination of internal coordinates for C_ℓ which gives the distance of $\mathbf{r}_i$ from the center of mass of the cluster C_ℓ.

To see how these definitions operate, let us consider the simplest nontrivial example:

Example (clustered Jacobi coordinates) Let $N = 5$ and consider the partition $D = \{C_1, C_2, C_3\}$, $C_1 = \{1, 2, 3\}$, $C_2 = \{4\}$, $C_3 = \{5\}$. Then

$$\begin{aligned} \mathbf{R}_1 &= (\mu_1 + \mu_2 + \mu_3)^{-1}(\mu_1 \mathbf{r}_1 + \mu_2 \mathbf{r}_2 + \mu_3 \mathbf{r}_3) \\ \xi_1^{(C_1)} &= \mathbf{r}_1 - \mathbf{r}_3, \qquad \xi_2^{(C_1)} = \mathbf{r}_2 - \mathbf{r}_3 \\ \mathbf{R}_2 &= \mathbf{r}_4, \qquad \mathbf{R}_3 = \mathbf{r}_5, \qquad \zeta_1 = \mathbf{R}_2 - \mathbf{R}_1 \\ \zeta_2 &= \mathbf{R}_3 - (\mu_1 + \mu_2 + \mu_3 + \mu_4)^{-1}[(\mu_1 + \mu_2 + \mu_3)\mathbf{R}_1 + \mu_4 \mathbf{R}_2] \end{aligned}$$

The clustered Jacobi coordinates are just $\langle \zeta_1, \zeta_2, \xi_1^{(C_1)}, \xi_2^{(C_1)} \rangle$. See Figure XI.8. As an example of how $\mathbf{r}_{ij} (i \in C_1, j \in C_2)$ appears, notice that

$$\mathbf{r}_4 - \mathbf{r}_3 = \zeta_1 + (\mu_1 + \mu_2 + \mu_3)^{-1}[\mu_1 \xi_1^{(C_1)} + \mu_2 \xi_2^{(C_1)}]$$

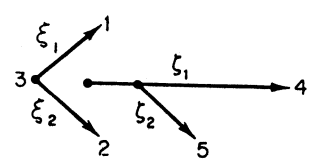


FIGURE XI.8 Clustered Jacobi coordinates, $N = 5$.

Having completed our discussion of the kinematics of N-body systems, we turn to the existence questions of scattering theory. We use the same technical ideas as in the two-body theory with the usual two complications. First, kinematics makes the notation more complex and the reader should keep a cool head; secondly, the wealth of scattering phenomena will require us to look at more objects than just s-$\lim_{t \to \mp\infty} e^{+iHt} e^{-iH_0 t}$. For suppose that $\psi = \lim_{t \to +\infty} e^{+iHt} e^{-iH_0 t} \varphi$. Then $e^{-iHt}\psi$ approaches $e^{-iH_0 t}\varphi$ as $t \to +\infty$ and it looks like a state with N freely moving particles. If we want to describe states that asymptotically look like bound clusters $C_1, \ldots, C_k$ moving freely, we want $e^{-iHt}\psi$ to look like $e^{-iAt}\psi$ where A describes bound clusters moving freely. A must therefore include the forces that bind the clusters but should not have the forces between clusters. Thus we will take $A = H_D$, $D = \{C_1, \ldots, C_k\}$ and study a particular limit.

Definition Let H be the Hamiltonian of an N-body system with center of mass removed. Let $D = \{C_1, \ldots, C_k\}$ be a cluster decomposition of $\{1, \ldots, N\}$. If $\Omega_D^{\pm} = \text{s-lim}_{t \to \mp\infty} e^{+iHt} e^{-iH_D t}$ exist, we say that the **clustered channel wave operators exist.**

Theorem XI.34 (Hack's theorem) Let

$$H = \sum_{i=1}^{N-1} (-2\mu_i)^{-1} \Delta_i + \sum_{i<j} V_{ij}(\mathbf{r}_{ij})$$

where each $V_{ij} \in L^2(\mathbb{R}^3) + L^p(\mathbb{R}^3)$ with $2 < p < 3$. Then the clustered channel wave operators $\Omega_D^{\pm}$ exist for each cluster decomposition D.

Proof The basic structure of the proof is exactly that of the second proof of Theorem XI.24. Choose a clustered Jacobi coordinate system with coordinates $\zeta_1, \ldots, \zeta_{k-1}; \xi_1^{(C_1)}, \ldots, \xi_{n_1-1}^{(C_1)}; \ldots \xi_{n_k-1}^{(C_k)}$ where $\{\xi^{(C_\ell)}\}$ is a family of internal coordinates for cluster C_ℓ and $\{\zeta\}$ are the Jacobi coordinates for the motion of the centers of mass of the clusters. Consider the set

$$\mathscr{D}_D = \{\varphi(\zeta_1, \ldots, \zeta_{k-1}) \eta_1(\xi^{(C_1)}) \cdots \eta_k(\xi^{(C_k)}) \mid \varphi \in \mathscr{S}(\mathbb{R}^{3k-3}),$$
$$\text{and} \quad \eta_\ell \in D(H(C_\ell)), \|\eta_\ell\| = 1\}$$

Finite linear combinations of vectors in $\mathscr{D}_D$ are dense, so we need only prove that $\lim_{t \to \mp\infty} e^{+iHt} e^{-iH_D t} \psi$ exists for all $\psi \in \mathscr{D}_D$.

By Cook's method, it is sufficient to show that

$$\left\| \frac{d}{dt} (e^{+iHt} e^{-iH_D t} \psi) \right\| = \|I_D e^{-iH_D t} \psi\|$$

is in $L^1(\pm 1, \pm\infty)$ for all $\psi \in \mathscr{D}_D$. Since I_D is a finite sum, it is enough to show $\|V_{ij} e^{-iH_D t} \psi\| \in L^1(\pm 1, \pm\infty)$ for each i, j with $\sim iDj$. Since each V_{ij} is a sum of two terms, one in L^2 the other in L^r, we can suppose V_{ij} is in either L^2 *or* L^r $(2 < r < 3)$ and use the triangle inequality to estimate the sum. Given i, j, we shall pick the Jacobi coordinates so that $\zeta_1 = R_a - R_b$ where $i \in C_a$, $j \in C_b$. Since change of Jacobi coordinates of $\langle R_1, \ldots, R_k \rangle$ by reordering leaves $\mathscr{S}(\mathbb{R}^{3k-3})$ invariant, there is no problem with the fact that we must change the meaning of "ζ_ℓ" as we vary i and j.

We next note that the individual terms in

$$H_D = \sum_{\ell=1}^{k-1} (-2M_\ell)^{-1} \Delta_\ell + \sum_{\ell=1}^{k} H(C_\ell)$$

commute, so

$$e^{-itH_D} = \left(\prod_{\ell=1}^{k-1} e^{+it(2M_\ell)^{-1} \Delta_\ell} \right) \prod_{\ell=1}^{k} e^{-itH(C_\ell)}$$

Moreover, V_{ij} depends only on ζ_1 and internal coordinates from C_1, C_2, so V_{ij} commutes with $e^{is\Delta_\ell}$, $\ell \neq 1$ and $e^{-itH(C_\ell)}$, $\ell \neq 1, 2$. Thus

$$\|V_{ij} e^{-itH_D} \psi\| = \left\| V_{ij} (e^{is\Delta_1} \varphi)(\eta_{1,t})(\eta_{2,t}) \prod_{\ell=3}^{k} \eta^{(C_\ell)} \right\|$$

where $s = t(2M_1)^{-1}$; and $\eta_{\ell,t} = e^{-iH(C_\ell)t} \eta_\ell$. V_{ij} depends only on ζ_1 and coordinates in C_1 and C_2, so

$$\|V_{ij} e^{-itH_D} \psi\| = \|V_{ij} (e^{is\Delta_1} \varphi)(\eta_{1,t})(\eta_{2,t})\|_{C_1, C_2; \zeta}$$

where the symbol $\|\cdot\|_{C_1, C_2; \zeta}$ means the L^2-norm integrating over the variables $\xi^{(C_1)}$, $\xi^{(C_2)}$, and ζ. Thus

$$\|V_{ij} e^{-itH_D} \psi\|^2 = \int F(\zeta_2, \ldots, \zeta_{k-1}; t) \, d\zeta_2 \cdots d\zeta_{k-1}$$

where

$$F(\zeta_2, \ldots, \zeta_{k-1}; t) = \int |V_{ij}^{(t)}(\zeta_1)|^2 |e^{is\Delta_1} \varphi(\zeta_1, \ldots, \zeta_{k-1})|^2 \, d\zeta_1$$

and

$$|V_{ij}^{(t)}(\zeta_1)|^2 = \int |\eta_{1,t}(\xi_1^{(C_1)})|^2 |\eta_{2,t}(\xi_1^{(C_2)})|^2 |V_{ij}(\zeta_1 - \xi_i^{(C_1)} - \xi_j^{(C_2)})|^2 \, d\xi^{(C_1)} \, d\xi^{(C_2)}$$

If we do all the $\xi^{(C_1)}$, $\xi^{(C_2)}$ integrations in the last integral except for the $\xi_i^{(C_1)} + \xi_j^{(C_2)}$ integration, we see that $|V_{ij}^{(t)}|^2$ is a convolution of $|V_{ij}|^2 \in L^{r/2}$ and a function in L^1 with L^1-norm $(\|\eta_{1,t}\|_2 \|\eta_{2,t}\|_2)^2 = 1$. Thus by Young's inequality, $\|V_{ij}^t\|_r \leq \|V_{ij}\|_r$. As a result of this estimate and the wave packet spreading of $e^{is\Delta_1}$, we conclude that

$$0 \leq F(\zeta_2, \ldots, \zeta_{k-1}) \leq \|V_{ij}^{(t)}\|_r^2 (s^{-\frac{1}{2}+3/p})^2 \int |\varphi(\zeta_1, \ldots, \zeta_{k-1})|^2 \, d\zeta_1$$

where p is as given in Theorem XI.24 and in particular $p > 6$. Finally, we conclude that

$$\|V_{ij} e^{-itH} \psi\|^2 \leq [\|V_{ij}\|_r s^{-\frac{1}{2}+3/p} \|\varphi\|_2]^2$$

and thus $\|V_{ij} e^{-itH} \psi\| \in L^1(\pm 1, \pm\infty)$. This concludes the proof. ∎

The point of the above proof is that it reduces the existence problem for the N-body case to the same estimates we used in the two-body case. By using the form ideas discussed in the proof of Theorem XI.26 and the form version of Cook's method (Theorem XI.6), one easily obtains:

Theorem XI.35 Let

$$H = \sum_{i=1}^{N-1} (-2\mu_i)^{-1}\Delta_i + \sum_{i<j} V_{ij}(r_{ij})$$

on $L^2(\mathbb{R}^{(N-1)n})$. Suppose that each V_{ij} obeys

$$(1 + |r|^2)^{\frac{1}{2}+\varepsilon} V_{ij}(r) \in L^p(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$$

where $p = \frac{1}{2}n$ if $n \geq 3$; $p = 1$ if $n = 1$; and $p > 1$ if $n = 2$. Then the clustered channel wave operators $\Omega_D^\pm$ exist for each cluster decomposition D.

We now know that $\Omega_D^\pm$ exist and would like to construct scattering states. Not every $\psi = \Omega_D^- \kappa$ describes a state that approaches a system of bound clusters $\{C_1, C_2, \ldots, C_k\}$ moving freely relative to one another as $t \to \infty$. All we know is that $e^{-iHt}\psi$ and $e^{-iH_D t}\kappa$ approach one another. But since $\text{s-lim}_{t\to\infty} e^{+iH_D t}e^{-iH_0 t}$ exists, if $\kappa = \lim_{t\to\infty} e^{+iH_D t}e^{-iH_0 t}\eta$, then $e^{-iHt}\psi$ and $e^{-iH_0 t}\eta$ also look like one another as $t \to \infty$. The point is that for ψ to look like bound clusters as $t \to \infty$, it is not enough to have $e^{-itH}\psi - e^{-itH_D}\kappa \to 0$ for an arbitrary κ. κ must have the form $\kappa(\zeta, \xi^{(C_1)}, \ldots, \xi^{(C_k)}) = \varphi(\zeta)\eta_1(\xi^{(C_1)}) \cdots \eta_k(\xi^{(C_k)})$ where each η_ℓ is a bound state of $H(C_\ell)$. We thus are motivated to define:

Definition A **channel** is a cluster decomposition $D = \{C_1, \ldots, C_k\}$ together with functions $\eta_\ell \in \mathscr{H}_{C_\ell}$ such that each η_ℓ is an eigenfunction of $H(C_\ell)$ with eigenvalue E_ℓ. We shall use the symbols α, β, ... to stand for a channel and sometimes write

$$\alpha = \begin{pmatrix} C_1 & C_2 & \cdots & C_k \\ \eta_1 & \eta_2 & \cdots & \eta_k \end{pmatrix}$$

The eigenvalues $E_1, \ldots, E_k$ will be denoted $\{E_i^{(\alpha)}\}_{i=1}^k$ and are called **channel eigenenergies**. The cluster decomposition D associated with a channel α will be denoted by $D(\alpha)$.

Two channels where the η_ℓ differ by complex multiples are not considered distinct. Thus a channel is more accurately a cluster decomposition together with "rays of eigenfunctions." If C_ℓ contains only one particle, then we write $\mathscr{H}_{C_\ell} = \mathbb{C}$ (there are no internal coordinates), $H(C_\ell) \equiv 0$, η_ℓ is the element $1 \in \mathbb{C}$, and $E_\ell^{(\alpha)} = 0$.

Important Proviso In listing all channels $\alpha = \binom{C_1 \cdots C_k}{\eta_1 \cdots \eta_k}$, we first make preliminary choices if some $H(C_\ell)$ has a degenerate eigenvalue. Explicitly, if E_0 is an eigenvalue of $H(C_\ell)$ of multiplicity n, we first pick n orthonormal functions in $\{\eta \,|\, H(C_\ell)\eta = E_0\eta\}$ and then require that for any α with $E_\ell^{(\alpha)} = E_0$, η_ℓ is one of these n functions. Thus if α and β are distinct channels, either $D(\alpha) \neq D(\beta)$ or $D(\alpha) = D(\beta)$ and for some ℓ, $\eta_\ell^{(\alpha)}$ is orthogonal to $\eta_\ell^{(\beta)}$.

Definition Let α be a channel. Choose clustered Jacobi coordinates for the decomposition $D(\alpha)$, say $\langle \zeta_1, \ldots, \zeta_{k-1}, \xi_1^{(C_1)}, \ldots, \xi_{n_k-1}^{(C_k)} \rangle$. Call $\mathscr{H}_\alpha = L^2(\mathbb{R}^{3k-3})$ the **channel Hilbert space**, and define $\mathscr{T}_\alpha : \mathscr{H}_\alpha \to \mathscr{H} = L^2(\mathbb{R}^{3N-3})$, **the channel embedding** by

$$(\mathscr{T}_\alpha \varphi)(\zeta, \xi^{(C_\ell)}) = \varphi(\zeta_1, \ldots, \zeta_{k-1}) \prod_{\ell=1}^k \eta_\ell(\xi^{(C_\ell)})$$

The **channel wave operators** $\Omega_\alpha^\pm : \mathscr{H}_\alpha \to \mathscr{H}$ are defined by

$$\Omega_\alpha^\pm = \Omega_{D(\alpha)}^\pm \mathscr{T}_\alpha$$

The **channel Hamiltonian** H_α on $\mathscr{H}_\alpha$ is defined by

$$H_\alpha = H_\alpha^{(0)} + \sum_{\ell=1}^k E_\ell^{(\alpha)}$$

where $H_\alpha^{(0)} = \sum_{\ell=1}^{k-1} (-2M_\ell)^{-1}\Delta_\ell$ in Jacobi coordinates.

The wave operators $\Omega_\alpha^\pm$ have a simple direct physical interpretation. For, if $\psi = \Omega_\alpha^\pm \varphi$, then $e^{-iHt}\psi$ approaches $(e^{-iH_\alpha^{(0)}t}\varphi)(\prod_{\ell=1}^k e^{-itE_\ell^{(\alpha)}}\eta_\ell)$ as $t \to \mp\infty$. But $(e^{-iH_\alpha^{(0)}t}\varphi)(\prod_{\ell=1}^k e^{-itE_\ell^{(\alpha)}}\eta_\ell)$ is precisely the wave function of bound clusters η_ℓ moving freely relative to one another. Given this physical interpretation, we expect that Ran $\Omega_\alpha^\pm$ should be orthogonal to Ran $\Omega_\beta^\pm$. We have thus removed the multiple counting of asymptotic states that occurs in $\{\text{Ran } \Omega_D^\pm\}$. Before proving that Ran $\Omega_\alpha^\pm$ and Ran $\Omega_\beta^\pm$ are orthogonal if $\alpha \neq \beta$, we combine the channels.

Definition Let $\mathscr{C}$ be the collection of all channels with the proviso discussed above in case some $H(C_\ell)$ has a degenerate eigenvalue. Define the **asymptotic Hilbert space** $\mathscr{H}_{\text{asym}} = \oplus_{\alpha\in\mathscr{C}} \mathscr{H}_\alpha$, the "**free**" **Hamiltonian** H_{asym}

on $\mathscr{H}_{\text{asym}}$ by $H_{\text{asym}} = \oplus_{\alpha \in \mathscr{C}} H_\alpha$, the **embedding transformation** $\mathscr{T}$: $\mathscr{H}_{\text{asym}} \to \mathscr{H}$ by $\mathscr{T} = \oplus_{\alpha \in \mathscr{C}} \mathscr{T}_\alpha$, and the **wave operators** $\Omega^\pm$: $\mathscr{H}_{\text{asym}} \to \mathscr{H}$ by $\Omega^\pm = \oplus_{\alpha \in \mathscr{C}} \Omega_\alpha^\pm$. Let $\mathscr{H}_\pm = \text{Ran}\, \Omega^\pm$.

Theorem XI.36 Suppose that the cluster channel wave operators exist. Then:

(a) $\Omega^\pm = \text{s-lim}_{t \to \mp\infty} e^{+iHt} \mathscr{T} e^{-iH_{\text{asym}}t}$.
(b) (Orthogonality of channels) If $\alpha \neq \beta$, then Ran $\Omega_\alpha^\pm$ is orthogonal to Ran $\Omega_\beta^\pm$.
(c) $\Omega^\pm$ are isometries from $\mathscr{H}_{\text{asym}}$ to $\mathscr{H}$.
(d) $e^{iHt}\Omega^\pm = \Omega^\pm e^{iH_{\text{asym}}t}$.
(e) $\mathscr{H}_\pm \subset \mathscr{H}_{\text{ac}}(H)$.

Proof (a) This is a direct consequence of $e^{-iH_{D(\alpha)}t}\mathscr{T}_\alpha = \mathscr{T}_\alpha e^{-iH_\alpha t}$.

(b) Let $\varphi_\alpha \in \mathscr{H}_\alpha$, $\varphi_\beta \in \mathscr{H}_\beta$. Then $\Omega_\alpha^\pm \varphi_\alpha = \text{s-lim}_{t \to \mp\infty} e^{+iHt}\mathscr{T}_\alpha e^{-iH_\alpha t}\varphi_\alpha$ and similarly for φ_β. Thus since e^{+iHt} is unitary, it is sufficient to prove that $\lim_{t \to \mp\infty} (\mathscr{T}_\alpha e^{-iH_\alpha t}\varphi_\alpha, \mathscr{T}_\beta e^{-iH_\beta t}\varphi_\beta) = 0$ in order to conclude that $(\Omega_\alpha^\pm \varphi_\alpha, \Omega_\beta^\pm \varphi_\beta) = 0$. This is done by considering separately the cases where $D(\alpha) = D(\beta)$ and $D(\alpha) \neq D(\beta)$.

First suppose that $D(\alpha) = D(\beta)$. Then

$$\begin{aligned}(\mathscr{T}_\alpha e^{-iH_\alpha t}\varphi_\alpha, \mathscr{T}_\beta e^{-iH_\beta t}\varphi_\beta) &= (e^{-iH_{D(\alpha)}t}\mathscr{T}_\alpha \varphi_\alpha, e^{-iH_{D(\beta)}t}\mathscr{T}_\beta \varphi_\beta) \\ &= (\mathscr{T}_\alpha \varphi_\alpha, \mathscr{T}_\beta \varphi_\beta) = \left(\varphi_\alpha \prod_{\ell=1}^{k} \eta_\ell^{(\alpha)}, \varphi_\beta \prod_{\ell=1}^{k} \eta_\ell^{(\beta)}\right) \\ &= (\varphi_\alpha, \varphi_\beta)\left[\prod_{\ell=1}^{k} (\eta_\ell^{(\alpha)}, \eta_\ell^{(\beta)})\right] = 0\end{aligned}$$

because some $(\eta_\ell^{(\alpha)}, \eta_\ell^{(\beta)}) = 0$ by our proviso on degenerate eigenvalues.

Now suppose that $D(\alpha) \neq D(\beta)$. Let $E = \sum_{\ell=1}^{k_\beta} E_\ell^{(\beta)} - \sum_{\ell=1}^{k_\alpha} E_\ell^{(\alpha)}$. Then

$$\begin{aligned}(\mathscr{T}_\alpha e^{-itH_\alpha}\varphi_\alpha, \mathscr{T}_\beta e^{-itH_\beta}\varphi_\beta) &= e^{-itE}(\mathscr{T}_\alpha e^{-itH_\alpha^{(0)}}\varphi_\alpha, \mathscr{T}_\beta e^{-itH_\beta^{(0)}}\varphi_\beta) \\ &= e^{-itE}(\mathscr{T}_\alpha \varphi_\alpha, e^{-it[H_\beta^{(0)} - H_\alpha^{(0)}]}\mathscr{T}_\beta \varphi_\beta)\end{aligned}$$

$H_\beta^{(0)} - H_\alpha^{(0)} \neq 0$ because $D(\alpha) \neq D(\beta)$. Written in terms of Fourier transforms, $H_\beta^{(0)} - H_\alpha^{(0)}$ is multiplication by some function $f_{\alpha\beta}(p)$ which is a quadratic form in p and so has the form $f_{\alpha\beta}(p) = \sum_{i=1}^{3N-3} a_i p_i^2$ for some coordinate system, with some $a_i \neq 0$. Renumber the p_i so that $a_1, \ldots, a_m \neq 0$; $a_{m+1} = a_{m+2} = \cdots = 0$. Let ψ_1 and ψ_2 be in $\mathscr{S}(\mathbb{R}^{3N-3})$. Then by (IX.31),

$$\begin{aligned}&(\psi_1, e^{-it(H_\beta^{(0)} - H_\alpha^{(0)})}\psi_2) \\ &\quad = \int \overline{\psi_1(x_1, \ldots, x_m, z_{m+1}, \ldots, z_{3N-3})}\, K(x, y) \\ &\qquad \times \psi_2(y_1, \ldots, y_m, z_{m+1}, \ldots, z_{3N-3})\, d^m x\, d^m y\, d^{3N-3-m} z\end{aligned}$$

with

$$K(x, y) = (-1)^\sigma t^{-m/2}(2\pi i)^{-m/2} \prod_{i=1}^{m} |a_i|^{-1/2} \exp(i|x_i - y_i|^2/4a_i t)$$

where σ depends on the number of negative a_i.

Because of the $t^{-m/2}$ factor, $(\psi_1, e^{-it(H_\beta^{(0)} - H_\alpha^{(0)})}\psi_2) \to 0$ as $t \to \infty$. By an $\varepsilon/3$ argument, $(\psi_1, e^{-it(H_\beta^{(0)} - H_\alpha^{(0)})}\psi_2) \to 0$ for all ψ_1, ψ_2 and in particular $(\mathscr{T}_\alpha \varphi_\alpha, e^{-it(H_\beta^{(0)} - H_\alpha^{(0)})}\mathscr{T}_\beta \varphi_\beta) \to 0$. This proves the orthogonality of channels.

(c) Let $\psi \in \mathscr{H}_{\text{asym}}$. Then $\Omega^\pm \psi = \sum_\alpha \Omega_\alpha^\pm \psi_\alpha$. Since the $\Omega_\alpha^\pm \psi_\alpha$ are orthogonal to one another,

$$\|\Omega^\pm \psi\|^2 = \sum_\alpha \|\Omega_\alpha^\pm \psi_\alpha\|^2 = \sum_\alpha \|\Omega_{D(\alpha)}^\pm \mathscr{T}_\alpha \psi_\alpha\|^2 = \sum \|\psi_\alpha\|^2 = \|\psi\|^2$$

where we have used the fact that each $\mathscr{T}_\alpha$ and each $\Omega_\alpha^\pm$ is isometric.

(d) and (e) are proven as is the two-body case. ∎

Notice that $\mathscr{T}$ is not an isometry, for the Ran $\mathscr{T}_\alpha$ are not orthogonal to one another. For example, Ran $\mathscr{T}_\alpha = \mathscr{H}$ if α is the unique channel with $D(\alpha) = \{\{1\}, \ldots, \{N\}\}$. The proof that $\Omega^\pm$ are isometric depended critically on the fact that Ran $\Omega_\alpha^\pm$ are orthogonal to Ran $\Omega_\beta^\pm$ if $\alpha \neq \beta$. This in turn was essentially a consequence of the fact that $\lim_{t \to \pm\infty} \|\mathscr{T} e^{-itH_{\text{asym}}}\psi\| = \|\psi\|$ for all ψ, which was proven in (b) above.

We now define the S-operator:

Definition Let S: $\mathscr{H}_{\text{asym}} \to \mathscr{H}_{\text{asym}}$ be the operator $S = (\Omega^-)^*\Omega^+$. S is called the ***S*-operator, *S*-matrix,** or scattering operator. We also define $S_{\alpha\beta}$: $\mathscr{H}_\beta \to \mathscr{H}_\alpha$ by $S_{\alpha\beta} = (\Omega_\alpha^-)^*\Omega_\beta^+$ so that $S = \sum_{\alpha,\beta} S_{\alpha\beta}$.

For example, let $N = 3$, suppose that β is the unique channel with $D(\beta) = \{\{1\}, \{2\}, \{3\}\}$ and that α is a channel with $D(\alpha) = \{\{1, 2\}, \{3\}\}$. Then $S_{\alpha\beta}$ describes a capture process and $S_{\beta\alpha}$ describes a breakup.

As usual,

Definition If $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^- = \mathscr{H}_{ac}(H)$, we say that the scattering for the N-body system is **complete.**

By rather involved methods, the following has been proven:

Theorem XI.37 Let $N = 3$, $\tilde{H} = \sum_{i=1}^{3} (-2m_i)^{-1}\Delta_i + \sum_{1\le i<j\le 3} V_{ij}$. Suppose that:

(i) Each V_{ij} obeys $V_{ij} \in L^{\frac{3}{2}+\varepsilon}(\mathbb{R}^3) \cap L^{\frac{3}{2}-\varepsilon}(\mathbb{R}^3)$ and $(1+|x|)^{2+\varepsilon}V_{ij} \in L^2 + L^\infty$. (Roughly speaking, $V_{ij}(x)$ is required to have $|x|^{-2-\varepsilon}$ falloff.)

(ii) No two-body subsystem has a "zero energy resonance or bound state" in the following exact sense: Let $\mu_{ij} = (m_i^{-1} + m_j^{-1})^{-1}$. Let $k_{ij}(\lambda) = -(2\mu_{ij})^{-1}\Delta + \lambda V_{ij}(x)$ on $L^2(\mathbb{R}^3)$. Then the dimension of the spectral projection onto $(-\infty, 0)$ for $k_{ij}(\lambda)$ is independent of λ for $|\lambda - 1| < \delta$ for some $\delta > 0$. Moreover, no $k_{ij}(1)$ has a positive eigenvalue.

Then $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^- = \mathscr{H}_{ac}(H)$.

For certain N-body systems with only one channel (that is, systems with no bound states for the $H(C)$), completeness has been proven; see Theorem XIII.27 for the case of weak coupling and Theorem XIII.32 for the case of repulsive potentials.

It seems likely that the methods of Section 17 will be extended to prove fairly strong results on asymptotic completeness for multiparticle Hamiltonians.

There is a final topic in the scattering of N-body systems which we would like to discuss, namely cluster properties of $\Omega^\pm$ and the related definition of the "connected part" of the S-matrix. These properties play a major role in further developments of N-body scattering, particularly in the physics literature. However, we caution the reader that the technical details are quite complicated and may be omitted since we shall not use these properties again. Cluster properties are simpler to express if we do not remove the center of mass motion. Thus let us define

$$\tilde{\mathscr{H}} = L^2(\mathbb{R}^3)\otimes\mathscr{H}, \qquad \tilde{\mathscr{H}}_{\text{asym}} = L^2(\mathbb{R}^3)\otimes\mathscr{H}_{\text{asym}}$$

$$\tilde{\Omega}_D^\pm = 1\otimes\Omega_D^\pm, \qquad \tilde{\Omega}_\alpha^\pm = 1\otimes\Omega_\alpha^\pm, \qquad \tilde{S} = 1\otimes S, \qquad \tilde{\mathscr{T}}_\alpha = 1\otimes\mathscr{T}_\alpha$$

$$\tilde{H} = h_0^{\text{CM}}\otimes 1 + 1\otimes H, \qquad \tilde{H}_{\text{asym}} = h_0^{\text{CM}}\otimes 1 + 1\otimes H_{\text{asym}}$$

Let i be in $\{1, \ldots, N\}$, $\mathbf{a}$ be in $\mathbb{R}^3$, and define $U^i(\mathbf{a})$ on $\tilde{\mathscr{H}}$ by:

$$(U^i(\mathbf{a})f)(\mathbf{x}_1, \ldots, \mathbf{x}_n) = f(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_i - \mathbf{a}, \ldots, \mathbf{x}_n)$$

Given a cluster decomposition $D = \{C_1, \ldots, C_k\}$ and $\mathbf{a}_1, \ldots, \mathbf{a}_k \in \mathbb{R}^3$ we define $U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$ on $\tilde{\mathscr{H}}$ by

$$U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = \Big(\prod_{i\in C_1} U^i(\mathbf{a}_1)\Big)\Big(\prod_{i\in C_2} U^i(\mathbf{a}_2)\Big)\cdots\Big(\prod_{i\in C_k} U^i(\mathbf{a}_k)\Big)$$

Thus $U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$ translates the clusters relative to one another. To state the major technical result, which we shall then interpret, we need some other notions:

Definition Let $D^{(1)}$ and $D^{(2)}$ be two cluster decompositions. We say $D^{(2)}$ **is a refinement** of $D^{(1)}$ and write $D^{(1)} \lhd D^{(2)}$ if each element $C_\ell^{(2)}$ of $D^{(2)}$ is a subset of some $C_j^{(1)}$ of $D^{(1)}$.

Thus D_2 is a refinement of D_1 if each cluster in D_1 is obtained by grouping together one or more clusters in D_2. We write $D_1 \lhd D_2$ to indicate that several sets in D_2 are joined to form the sets in D_1.

If D is a cluster decomposition, there is associated a natural tensor product decomposition of $\tilde{\mathscr{H}}$ into $\otimes_{\ell=1}^k \tilde{\mathscr{H}}_{C_\ell}$ where $\tilde{\mathscr{H}}_{C_\ell}$ is the space of functions of the coordinates $\{\mathbf{r}_i \mid i \in C_\ell\}$. Suppose $D \lhd D'$. Then for each $C_\ell \in D$, D' induces a cluster decomposition D'_ℓ of C_ℓ by taking the family of elements of D' contained in C_ℓ. In such a case we write $\tilde{\Omega}_{D'_\ell}^\pm$ as the cluster channel wave operator on $\tilde{\mathscr{H}}(C_\ell)$ associated with the cluster D'_ℓ. Thus,

$$\tilde{\Omega}_{D'}^\pm = \operatorname*{s-lim}_{t\to\mp\infty} \exp(it\tilde{H}(C_\ell))\exp\Big(-it\sum_{C_j'\subset C_\ell}\tilde{H}(C_j')\Big)$$

Theorem XI.38 Let $V_{ij} \in L^2(\mathbb{R}^3) + L^r(\mathbb{R}^3)$, $2 < r < 3$,

(a) If $D < D'$, then

$$\operatorname*{s-lim}_{\min_{i\neq j}|\mathbf{a}_i-\mathbf{a}_j|\to\infty} U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)^{-1}\tilde{\Omega}_{D'}^\pm U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = \bigotimes_{\ell=1}^k \tilde{\Omega}_{D'_\ell}^\pm$$

(b) If $D \lhd D'$, then

$$\operatorname*{s-lim}_{\min_{i\neq j}|\mathbf{a}_i-\mathbf{a}_j|\to\infty} U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)^{-1}(\tilde{\Omega}_{D'}^\pm)^* U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = \bigotimes_{\ell=1}^k (\tilde{\Omega}_{D'_\ell}^\pm)^*$$

(c) If $D \not\lhd D'$ and β is any channel with $D(\beta) = D'$, then

$$\operatorname*{s-lim}_{\min_{i\neq j}|\mathbf{a}_i-\mathbf{a}_j|\to\infty} (\tilde{\Omega}_\beta^\pm)^* U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = 0$$

Proof The proof of (a) is essentially identical to the proof of Theorem XI.33, so we sketch the major ideas leaving the details to the reader (Problem 54). One first notes that

$$U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) \bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D_\ell} = \bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D_\ell} U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$$

since $\prod_{i \in \mathscr{C}_\ell} U^i(\mathbf{a}_\ell)$ commutes with $\tilde{\Omega}^{\pm}_{D_\ell}$, and that

$$\bigotimes_{i=1}^{k} \tilde{\Omega}^{\pm}_{D_\ell} = \text{s-lim}_{t \to \mp\infty} e^{+iH_D t} e^{-iH_{D'} t}$$

Thus

$$\tilde{\Omega}^{\pm}_{D'} = \left(\text{s-lim}_{t \to \mp\infty} e^{+iHt} e^{-iH_D t}\right)\left[\bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D_\ell}\right] = \tilde{\Omega}^{\pm}_{D}\left[\bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D_\ell}\right]$$

so to prove that $U_D^{-1}(\tilde{\Omega}^{\pm}_{D'} - \bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D_\ell}) U_D$ goes strongly to 0, we need only prove that

$$\text{s-lim}_{\min_{i \neq j} |\mathbf{a}_i - \mathbf{a}_j| \to \infty} U_D^{-1}(\mathbf{a})[\tilde{\Omega}^{\pm}_{D} - 1] U_D(\mathbf{a}) = 0 \tag{75}$$

But, for $\varphi \in D(H_0)$,

$$(\tilde{\Omega}^{\pm}_{D} - 1)\varphi = i \int_0^{\mp\infty} (e^{+iHt} I_D e^{-iH_D t} \varphi)\, dt$$

One proceeds now as we did in Theorem XI.33, using the estimates in Theorem XI.34 in place of those in Theorem XI.24. We defer the proof of (b) until after we prove (c).

(c) The heuristics behind this are that $(\Omega^{\pm}_{\beta})^*$ is zero on those states that asymptotically fail to form bound clusters in D'. Since $D \not\prec D'$, there is some pair $\langle i, j \rangle$ with $iD'j$ but $\sim iDj$. Thus $U_D(\mathbf{a})$ pries apart some cluster in D' as $\min |\mathbf{a}_i - \mathbf{a}_j| \to \infty$ and prevents $U_D \psi$ from being a state that forms bound clusters in D'. This heuristic argument really has two elements; first U_D "pries apart clusters in D'," so we shall show that

$$\text{s-lim}_{\min |\mathbf{a}_i - \mathbf{a}_j| \to \infty} \mathscr{J}^*_{\beta} U_D(\mathbf{a}) = 0 \tag{76}$$

Secondly, $e^{-iHt} U_D(\mathbf{a})$ approaches $e^{-iH_D t} U_D(\mathbf{a})$ strongly as $\min |\mathbf{a}_i - \mathbf{a}_j| \to \infty$; that is, as the clusters in D are moved apart, the part of the dynamics due to forces between the clusters becomes negligible.

As usual, to prove (76) it is enough to show that $\mathscr{J}^*_{\beta} U_D(a)\psi \to 0$ for a set of ψ whose linear combinations are dense in $\mathscr{H}$. Let $D' = \{C'_1, \ldots, C'_{k'}\}$ and pick $\psi = \varphi_1 \cdots \varphi_{k'}$ where φ_i is a function of the coordinates in C'_i. For each j, let $i(j)$ be that number so that $j \in C'_i$, one of the clusters of D. Suppose that

$$\beta = \begin{pmatrix} C'_1 & \cdots & C'_{k'} \\ \eta_1 & \cdots & \eta'_{k'} \end{pmatrix}$$

Thus,

$$\|\mathscr{J}^*_{\beta} U_D(a)\psi\|_{\mathscr{H}_\beta} = \prod_{\ell=1}^{k'} \left\| \int \eta_\ell(\xi^{(C_{\ell'})}) \varphi(\{r_i + a_{i(j)}\}_{j \in C_{\ell'}})\, d\xi^{(C_{\ell'})} \right\|_{\mathscr{H}(C_{\ell'})}$$

The point is that in some C'_ℓ, there are j_1, j_2 with $i(j_1) \neq i(j_2)$. Thus, when the coordinates $\mathbf{r}_j + \mathbf{a}_{i(j)}$ in φ_ℓ are changed to $\mathbf{R}_\ell$, $\xi^{(C_{\ell'})}$ coordinates, some ξ's are translated as well as $\mathbf{R}_\ell$. Since we are taking an inner product in ξ with a fixed η, the norm $\| \cdots \|_{\mathscr{H}(C_{\ell'})}$ will go to zero, so (76) is proven.

Next we prove that

$$\text{s-lim}_{\min |\mathbf{a}_i - \mathbf{a}_j| \to \infty} (e^{-iHt} - e^{-iH_D t}) U_D(\mathbf{a}) = 0 \tag{77a}$$

and

$$\text{s-lim}_{\min |\mathbf{a}_i - \mathbf{a}_j| \to \infty} (e^{+iH_{D'} t} - e^{+iH_{D' * D} t}) U_D(\mathbf{a}) e^{-iH_D t} = 0 \tag{77b}$$

uniformly in t where $D' * D$ is the cluster decomposition whose elements are $\{C'_\ell \cap C_m\}$ when $1 \leq \ell \leq k'$, $1 \leq m \leq k$. This is just an expression of the fact that if we apply $U_D(\mathbf{a})$ to a vector ψ, thereby prying the clusters in D apart, interactions between clusters make negligible contributions to the dynamics. If $\psi \in D(H_0)$, then

$$(e^{-iHt} - e^{-iH_D t}) U_D \psi = -ie^{-iHt} \int_0^t e^{+iHs} I_D e^{-iH_D s} U_D \psi\, ds$$

Thus to prove (77a) it is sufficient to prove that

$$\lim_{\min |\mathbf{a}_i - \mathbf{a}_j| \to \infty} \int_0^t \|I_D e^{-iH_D s} U_D(\mathbf{a})\psi\|\, ds = 0$$

uniformly in t. This is precisely the estimate we used in proving (75). To prove (77b), we need to prove that

$$\lim_{\min |\mathbf{a}_i - \mathbf{a}_j| \to \infty} \int_0^t \|(I_{D'} - I_{D * D'}) e^{iH_{D * D'} s} U_D(\mathbf{a}) e^{-iH_0 s} \psi\|\, ds = 0$$

uniformly in t, and this is proven in a similar way (Problem 55).

Now we can put (76) and (77) together to obtain the desired result. From (77) and the relations

$$U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)e^{-iH_0t} = e^{-iH_0t}U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$$
$$U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)e^{-iH_{D\cdot D'}t} = e^{-iH_{D\cdot D'}t}U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$$

one obtains that for any $\psi \in \mathscr{H}$,

$$\sup_{t\in\mathbb{R}} \|(e^{iH_{D'}t}e^{-iHt} - e^{iH_{D\cdot D'}t}e^{-iH_Dt})U_D\psi\| \to 0 \tag{78}$$

as $\min_{i\neq j}|\mathbf{a}_i - \mathbf{a}_j| \to \infty$. Let $\tilde{\Omega}^{\pm}_{D;\,D\cdot D'} = \text{s-lim}_{t\to\mp\infty} e^{iH_Dt}e^{-iH_{D\cdot D'}t}$ which exists by Theorem XI.34. Then

$$(\tilde{\Omega}^{\pm}_{D'} - \tilde{\Omega}_{D;\,D\cdot D'})^*U_D(\mathbf{a})\psi = \text{w-lim}_{t\to\mp\infty}\,(e^{iH_{D'}t}e^{-itH} - e^{iH_{D'\cdot D}t}e^{-iH_{D'}t})U_D(\mathbf{a})\psi$$

for each fixed ψ and $\mathbf{a}$. From the fact that $\|\text{w-lim}_{t\to\pm\infty}\psi_t\| \leq \lim_{t\to\pm\infty}\|\psi_t\|$, and (78) it follows that

$$\lim_{\min|\mathbf{a}_i-\mathbf{a}_j|\to\infty} \|(\tilde{\Omega}^{\pm}_{D'} - \tilde{\Omega}^{\pm}_{D,\,D\cdot D'})^*U_D(a)\psi\| = 0$$

Finally, since $(\tilde{\Omega}^{\pm}_{D,\,D\cdot D'})^*U_D(\mathbf{a}) = U_D(\mathbf{a})(\tilde{\Omega}^{\pm}_{D,\,D\cdot D'})^*$, we conclude

$$\text{s-lim}_{\min|\mathbf{a}_i-\mathbf{a}_j|\to\infty} \mathscr{T}^*_\beta(\tilde{\Omega}^{\pm}_{D'})^*U_D(\mathbf{a}) = \text{s-lim}_{\min|\mathbf{a}_i-\mathbf{a}_j|\to\infty} \mathscr{T}^*_\beta U_D(\mathbf{a})(\tilde{\Omega}^{\pm}_{D;\,D\cdot D'})^* = 0$$

This proves (c).

(77) holds whether $D \lhd D'$ or not, so its consequence s-lim $\|(\tilde{\Omega}^{\pm}_{D'} - \tilde{\Omega}^{\pm}_{D,\,D\cdot D'})^*U_D(\mathbf{a})\psi\| = 0$ holds. If $D \lhd D'$, then $D * D' = D'$ and $\tilde{\Omega}^{\pm}_{D,\,D\cdot D'} = \bigotimes_{\ell=1}^k \Omega^{\pm}_{D_\ell}$. This fact and $U_D^{-1}(\bigotimes_{\ell=1}^k \tilde{\Omega}^{\pm}_{D_\ell})^*U_D = (\bigotimes_{\ell=1}^k \tilde{\Omega}^{\pm}_{D_\ell})^*$ imply the result in (b). ∎

Now we use these cluster properties to obtain information about the S-operator. Let α be a channel and D a cluster decomposition with $D \lhd D(\alpha)$. In D some of the bound fragments in channel α are clumped together. This clumping induces a breakup of α into *subchannels*; namely, for each $C_\ell \in D$, let α_ℓ be the collection of clusters $F_m \in D(\alpha)$ with $F_m \subset C_\ell$ together with the bound states η_m in α. Thus, if $D = \{\{1, 2\}, \{3, 4, 5\}, \{6\}\}$ and

$$\alpha = \begin{pmatrix} \{1\} & \{2\} & \{3, 4\} & \{5\} & \{6\} \\ 1 & 1 & \varphi(\mathbf{r}_{34}) & 1 & 1 \end{pmatrix}$$

where $\varphi(\mathbf{r}_{34})$ is some bound state of $H(\{3, 4\})$, then

$$\alpha_1 = \begin{pmatrix} \{1\} & \{2\} \\ 1 & 1 \end{pmatrix}, \qquad \alpha_2 = \begin{pmatrix} \{3, 4\} & \{5\} \\ \varphi(\mathbf{r}_{34}) & 1 \end{pmatrix}, \qquad \alpha_3 = \begin{pmatrix} \{6\} \\ 1 \end{pmatrix}$$

The collection $\{\alpha_\ell\}_{\ell=1}^k$ is called the **decomposition of α induced by D**. Let $D = \{C_1, \ldots, C_k\}$ and let α, β be channels with $D \lhd D(\beta)$, $D \lhd D(\alpha)$. Let $\{\alpha_\ell\}_{\ell=1}^k$ and $\{\beta_\ell\}_{\ell=1}^k$ be the decompositions of α and β induced by D. Then we shall write $S^{(C_\ell)}_{\alpha_\ell,\beta_\ell}$ for the S-operator for the n_ℓ-body system which describes scattering from α_ℓ to β_ℓ.

Now let $D \lhd D(\alpha)$. Then $U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$ leaves Ran $\mathscr{T}_\alpha$ invariant and so induces a map $U^{(\alpha)}_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$ on $\tilde{\mathscr{H}}_\alpha$ by $U_D\mathscr{T}_\alpha = \mathscr{T}_\alpha U^{(\alpha)}_D$. Specifically, if $\varphi \in \tilde{\mathscr{H}}_\alpha$ is a function of $\langle \mathbf{r}_{F_1}, \ldots, \mathbf{r}_{F_m}\rangle$ where $D(\alpha) = \{F_1, \ldots, F_m\}$, then $U^{(\alpha)}_D$ acts on $\tilde{\mathscr{H}}_\alpha$ by translating those F_m in C_ℓ by $\mathbf{a}_\ell$. Fix $\psi \in \tilde{\mathscr{H}}_\alpha$ and consider the states $U^{(\alpha)}_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)\psi$ as $\min_{i\neq j}|\mathbf{a}_i - \mathbf{a}_j| \to \infty$. How do we expect $\tilde{S}U^\alpha_D\psi$ to behave? Let β be a channel with $D \not\lhd D(\beta)$. Then to scatter into β from α, particles in different clusters $C_\ell \in D$ must come together. Since the clusters in D are far apart in $U^\alpha_D\psi$, we expect no scattering into β. On the other hand, if $D \lhd D(\beta)$, one can scatter into β by scattering separately into each $C_\ell \in D$. We expect $\tilde{S}U^{(\alpha)}_D\psi$ to factor into separate scattering for each cluster C_ℓ. This is in fact true.

Theorem XI.39 (spatial cluster properties of S) Let α be a channel of an N-body quantum system that obeys the hypotheses of Theorem XI.34. Let D be a cluster decomposition with $D \lhd D(\alpha)$.

(a) If $D \lhd D(\beta)$, then

$$\text{s-lim}_{\min_{i\neq j}|\mathbf{a}_i-\mathbf{a}_j|\to\infty} \left(\tilde{S}_{\beta\alpha} - \bigotimes_{\ell=1}^k \tilde{S}^{(C_\ell)}_{\beta_\ell\alpha_\ell}\right) U^{(\alpha)}_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = 0$$

(b) If $D \not\lhd D(\beta)$, then

$$\text{s-lim}_{\min_{i\neq j}|\mathbf{a}_i-\mathbf{a}_j|\to\infty} \tilde{S}_{\beta\alpha}U^{(\alpha)}_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = 0$$

Proof To prove (a), we use Theorem XI.38a and b to first see that

$$\text{s-lim}\left(\tilde{S}_{\beta\alpha}U^{(\alpha)}_D - \mathscr{T}^*_\beta U_D \bigotimes_{\ell=1}^k \tilde{\Omega}^-_{D(\beta_\ell)}\tilde{\Omega}^+_{\alpha_\ell}\right) = 0$$

for

$$\tilde{S}_{\beta\alpha}U^{(\alpha)}_D - (\tilde{\Omega}^-_\beta)^*\left[U_D\bigotimes_{\ell=1}^k \tilde{\Omega}^+_{\alpha_\ell}\right] = (\tilde{\Omega}^-_\beta)^*\left[\tilde{\Omega}^+_\alpha U^{(\alpha)}_D - U_D\bigotimes_{\ell=1}^k \tilde{\Omega}^+_{\alpha_\ell}\right]$$

goes to zero strongly by Theorem XI.38a and similarly,

$$(\Omega_\beta^-)^*\left[U_D \bigotimes_{\ell=1}^{k} \tilde{\Omega}_{\alpha_\ell}^+\right] - \mathscr{F}_\beta^* U_D \bigotimes_{\ell=1}^{k} \tilde{\Omega}_{D(\beta\ell)}^- \tilde{\Omega}_{\alpha\ell}^+$$

$$= \mathscr{F}_\beta^*\left[(\tilde{\Omega}_{D(\beta)}^-)^* U_D - U_D \bigotimes_{\ell=1}^{k} (\tilde{\Omega}_{D(\beta)}^-)^*\right] \bigotimes_{\ell=1}^{k} \tilde{\Omega}_{\alpha_\ell}^+$$

goes to zero strongly by Theorem XI.38b. Finally, we remark that

$$\left(\bigotimes_{\ell=1}^{k} \mathscr{F}_{\beta\ell}^* \tilde{\Omega}_{D(\beta\ell)}^- \tilde{\Omega}_{\alpha\ell}^+\right) U_D^{(\alpha)} = \bigotimes_{\ell=1}^{k} \tilde{S}_{\beta_\ell \alpha_\ell}^{(C_\ell)} U_D^{(\alpha)}$$

To prove (b), we use Theorem XI.38c in place of Theorem XI.38b. ∎

Corollary If the S-matrix of an N-body quantum system obeying the hypotheses of Theorem XI.34 is unitary, then the S-matrix of any subsystem is unitary.

These spatial cluster properties are interesting because of their direct physical interpretation, but they are more important because of the "p-space smoothness" which they suggest. To understand the phenomenon which we are discussing, let us first consider two-body scattering. The $\tilde{S}$-operator is given by a kernel. One way of seeing this is to note that if $\varphi, \psi \in \mathscr{S}(\mathbb{R}^6)$, then $\langle \bar{\varphi}, \psi \rangle \to (\varphi, \tilde{S}\psi)$ is bilinear and continuous on $\mathscr{S}$ so there is a distribution $Q(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_3, \mathbf{x}_4)$ in $\mathscr{S}'(\mathbb{R}^{12})$ with

$$(\varphi, \tilde{S}\psi) = \int \overline{\varphi(\mathbf{x}_1, \mathbf{x}_2)} Q(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_3, \mathbf{x}_4) \psi(\mathbf{x}_3, \mathbf{x}_4)\, d^3x_1 \cdots d^3x_4$$

It is useful to write $\tilde{S}$ in p-space, that is, to look at the kernel of $\mathscr{F}\tilde{S}\mathscr{F}^{-1}$ where $\mathscr{F}$ is the Fourier transform:

$$(\varphi, \tilde{S}\psi) = \int \overline{\hat{\varphi}(p_1, p_2)} s(p_1, p_2; p_3, p_4) \hat{\psi}(p_3, p_4)\, d^3p_1 \cdots d^3p_4$$

Because of conservation of energy and momentum, that is, because S commutes with space translations and the *free* dynamics, the distribution s has support on the manifold where

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4$$

$$E_{\text{out}} \equiv \frac{\mathbf{p}_1^2}{2\mu_1} + \frac{\mathbf{p}_2^2}{2\mu_2} = \frac{\mathbf{p}_3^2}{2\mu_3} + \frac{\mathbf{p}_4^2}{2\mu_4} \equiv E_{\text{in}}$$

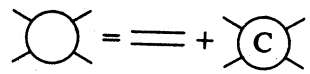
This suggests that s may be written in the form:

$$s(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_3, \mathbf{p}_4) = \delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4)\delta(E_{\text{in}} - E_{\text{out}}) s^{\text{red}}(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_4)$$

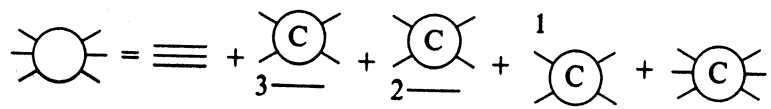
A priori, s could have much more complicated singularities such as $-\Delta\delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4)$. That such a δ-function singularity factors out is something we shall see when we discuss the reduction of the S-matrix by symmetries in Section 8. One might hope that s^{red} is a smooth function of the variables $\mathbf{p}_1, \ldots, \mathbf{p}_4$ as long as we vary them on the manifold where energy and momentum are conserved. This is not a good conjecture however! For let $U(\mathbf{a})$ be translation of the first particle by $\mathbf{a}$. Then $U(\mathbf{a})\tilde{S}U(\mathbf{a})^{-1}$ has a kernel $se^{i\mathbf{a}\cdot(\mathbf{p}_1 - \mathbf{p}_3)}$. If s^{red} were smooth, the Riemann–Lebesgue lemma would imply that $\lim_{\mathbf{a}\to\infty} (\varphi, U(\mathbf{a})\tilde{S}U(\mathbf{a})^{-1}\psi) = 0$, but we know that $\lim_{\mathbf{a}\to\infty} (\varphi, U(\mathbf{a})(\tilde{S} - I)U(\mathbf{a})^{-1}\psi) = 0$. This suggests that $\tilde{S} - I$ should have a smooth kernel; that is, we hope that

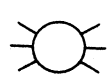
$$s(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_3, \mathbf{p}_4) = \delta(\mathbf{p}_1 - \mathbf{p}_3)\delta(\mathbf{p}_2 - \mathbf{p}_4) - (2\pi i)\delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4)\delta(E_{\text{in}} - E_{\text{out}}) t(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_3, \mathbf{p}_4)$$

where t is a smooth function of $\mathbf{p}_i$ if we vary $\langle \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_4 \rangle$ staying on the manifold where momentum and energy are conserved. The $\delta(\mathbf{p}_1 - \mathbf{p}_2)\delta(\mathbf{p}_3 - \mathbf{p}_4)$ term is just the kernel of the operator I. We put in the $2\pi i$ factor for conventional reasons. In the two-body case, we shall actually prove that s has this form for a wide variety of potentials; see Sections 6 and 7. What can we expect in the N-body case? Write the two-body result schematically



where  stands for the part with a smooth kernel; this part is called the "connected" part. One might guess for the three-body case:



so we can define  recursively in terms of  and the connected parts for fewer particles.

Definition Let α, β be channels of an N-body system. Define $R_{\alpha\beta}$ recursively (in N) by

$$R_{\alpha\beta} = \tilde{S}_{\alpha\beta} - \sum_{D \in \mathscr{D}_{\alpha\beta}} R_{\alpha_1\beta_1} \cdots R_{\alpha_k\beta_k}$$

where $\mathscr{C}_{\alpha,\beta}$ is the set of cluster decompositions with $D \lhd D(\alpha)$, $D \lhd D(\beta)$ *for which* D *contains at least two clusters.* For $N = 2$, $R = S - I$.

The spatial cluster properties of Theorem XI.39 then imply (Problem 56):

Theorem XI.40 (spatial cluster property of the reduced S-operators)

(a) $$\tilde{S}_{\alpha\beta} = \sum_{\substack{D \lhd D(\alpha),\ D \lhd D(\beta) \\ D = \{C_1, \ldots, C_k\}}} R_{\alpha_1\beta_1} R_{\alpha_2\beta_2} \cdots R_{\alpha_k\beta_k}$$

(b) $$\text{s-lim}_{\min_{i\neq j}|a_i - a_j| \to \infty} R_{\alpha\beta} U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = 0 \qquad \text{for all } D$$

with $D \lhd D(\beta)$.

This *suggests* that $R_{\alpha\beta}$ has a kernel of the form

$$r_{\alpha\beta}(\mathbf{p}, \mathbf{p}') = (2\pi i)\, \delta\left(\sum_{i=1}^{N} \mathbf{p}_i - \sum_{i=1}^{N} \mathbf{p}_i'\right) \delta(E - E') t_{\alpha\beta}(\mathbf{p}, \mathbf{p}')$$

where $t_{\alpha\beta}$ is a smooth function of $\mathbf{p}, \mathbf{p}'$. In fact, the "hypothesis of the analytic S-matrix" demands that $t_{\alpha\beta}(\mathbf{p}, \mathbf{p}')$ be the boundary value of a function analytic in certain regions. Unfortunately, this attractive hypothesis has not been proven in many-channel, many-body systems. In the Notes we shall discuss those results that constitute a partial proof of the "hypothesis of the analytic S-matrix" for quantum systems with $N \geq 3$.

XI.6 Quantum scattering III: Eigenfunction expansions

Any formal manipulations that are not obviously wrong are assumed to be correct.
M. L. Goldberger and K. Watson in **Scattering Theory**

For two-body quantum systems with potentials having $|x|^{-1-\varepsilon}$ falloff as $|x| \to \infty$, we have established the existence and uniqueness of scattering states. Completeness will be proven in Sections 17 and XIII.8. We have not, however, discussed any way of explicitly "computing" the S-operator or of correlating experimental data with the theory. Our goal in this section is to establish certain formulas which normally go under the name "formal scattering theory" or "time-independent scattering theory." These formulas present the S-operator as an explicit "integral operator" with kernel

$\delta(\mathbf{k} - \mathbf{k}') - 2\pi i\, \delta(k^2 - k'^2) T(\mathbf{k}, \mathbf{k}')$; see Theorem XI.42. In the next section we shall prove that the function $T(\mathbf{k}, \mathbf{k}')$ has an analytic continuation into certain regions.

The main tool in "formal scattering theory" is an eigenfunction expansion for the Hamiltonian H which is of considerable interest for its own sake. An operator A on $L^2(\mathbb{R}^3, dx)$ with purely discrete spectrum has an eigenfunction expansion in the direct sense that there are L^2 functions $\varphi_n(x)$ with an associated map $\tilde{}: L^2(\mathbb{R}^3, dx) \to \ell_2$ by

$$(\tilde{f})_n = \int \overline{\varphi_n(x)} f(x)\, dx \tag{79a}$$

That the φ_n are eigenfunctions with $A\varphi_n = a_n \varphi_n$ can be expressed by

$$(\widetilde{Af})_n = a_n \tilde{f}_n \qquad \text{if } f \in D(A) \tag{79b}$$

The orthonormality of the $\{\varphi_n\}$ implies

$$\text{Ran } \tilde{} = \ell_2 \tag{79c}$$

The completeness of the φ_n is expressed by

$$f(x) = L^2\text{-lim} \sum_{n=0}^{\infty} \tilde{f}_n \varphi_n(x) \tag{79d}$$

Finally, as a consequence of completeness and orthonormality:

$$\|f\|^2 = \sum_n |\tilde{f}_n|^2 \tag{79e}$$

Two-body Hamiltonians with center of mass removed have lots of spectrum that is nondiscrete—in fact, there is absolutely continuous spectrum $[0, \infty)$ associated with scattering. However, we can hope that some sort of "continuum" eigenfunction expansion exists. As a model of what we are seeking, we shall show how the Fourier transform provides an eigenfunction expansion for $H_0 = -\Delta$ which has only continuous spectrum. Write $\varphi_0(x, k) = e^{ik \cdot x}$ and think of $\varphi_0(\cdot, k)$ as a family of functions of x parametrized by a continuous index k. Then, we know that $\hat{}$ satisfies

$$\hat{f}(k) = (2\pi)^{-n/2}\, \text{l.i.m.} \int \overline{\varphi_0(x, k)} f(x)\, dx \tag{80a}$$

where l.i.m. $\int = L^2\text{-lim} \int_{|x|<M}$ as $M \to \infty$. The $\varphi_0(\cdot, k)$ are eigenfunctions with eigenvalue k^2 in the sense that

$$(\widehat{H_0 f})(k) = k^2 \hat{f}(k) \qquad \text{if } f \in D(H_0) \tag{80b}$$

The orthogonality and "normalization" of the $\varphi_0(\cdot, k)$ imply

$$\text{Ran } \hat{} = L^2(\mathbb{R}^3, dx) \tag{80c}$$

The completeness of the set $\{\varphi_0(\cdot, k)\}_{k \in \mathbb{R}^3}$ is expressed by

$$f(x) = \text{l.i.m. } (2\pi)^{-3/2} \int \varphi_0(x, k)\hat{f}(k)\, dk \tag{80d}$$

and

$$\|f\|^2 = \int |\hat{f}(k)|^2\, dk \tag{80e}$$

How can we find candidates φ for the "continuum eigenfunctions" needed for an eigenfunction expansion of $H = H_0 + V$? $\Omega^+ f$ has been defined only for $f \in L^2$, but suppose that we could make sense out of $\Omega^+\varphi_0(\cdot, k)$. Then, since $\Omega^+ H_0 = H\Omega^+$, $\varphi(\cdot, k) \equiv \Omega^+\varphi_0(\cdot, k)$ should obey $H\varphi = k^2\varphi$ in the sense of (80b). If $\varphi = \Omega^+\varphi_0$ in some sense, then $\varphi_0 = (\Omega^+)^*\varphi$ should be the limit as $t \to -\infty$ of

$$\begin{aligned} e^{+iH_0t}e^{-iHt}\varphi &= \varphi - i\int_0^t e^{iH_0s}Ve^{-iHs}\varphi\, ds \\ &\to \varphi - \lim_{\varepsilon \downarrow 0} i\int_0^{-\infty} e^{iH_0s}Ve^{-ik^2s}e^{+\varepsilon s}\varphi\, ds \\ &= \varphi + \lim_{\varepsilon \downarrow 0} (H_0 - k^2 - i\varepsilon)^{-1}V\varphi \end{aligned}$$

Thus φ should obey

$$\varphi(\cdot, k) = \varphi_0(\cdot, k) - \lim_{\varepsilon \downarrow 0} ([H_0 - (k^2 + i\varepsilon)]^{-1}V\varphi)(\cdot, k) \tag{81a}$$

or, using (IX.30),

$$\varphi(\mathbf{x}, \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{4\pi}\int \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|} V(\mathbf{y})\varphi(\mathbf{y}, \mathbf{k})\, d\mathbf{y} \tag{81b}$$

Physicists call Ω^+ the wave operator as $t \to -\infty$ because of the $+i\varepsilon$ in (81a). (81), an equation that we arrived at by heuristic argument, is known as the **Lippmann–Schwinger equation**. To find candidates φ for an eigenfunction expansion, we shall solve this equation. Once we have φ, we shall form the eigenfunction transform $f^*(k) = \text{l.i.m.}(2\pi)^{-3/2} \int \overline{\varphi(x, k)} f(x)\, dx$. We expect analogues of (80) to hold with one exception: The $\varphi(\cdot, k)$ will not in general be complete; that is, we no longer expect

$$f(x) = \text{l.i.m.}(2\pi)^{-3/2} \int f^*(k)\varphi(x, k)\, dk$$

since the φ's are only eigenfunctions associated with the absolutely continuous spectrum of H. Indeed, we shall find that $(P_{ac}(H)f)(x) = \text{l.i.m.}(2\pi)^{-3/2} \int f^*(k)\varphi(x, k)\, dk$. Finally, we expect that this eigenfunction transform and the Fourier transform should be related; for formally $\Omega^+\varphi_0 = \varphi$, which suggests that $\Omega^+(\int b(k)\varphi_0(x, k)\, dk) = \int b(k)\varphi(x, k)\, dk$ or that $(\Omega^+ f)^* = \hat{f}$ where we let $\hat{f} = (2\pi)^{3/2}b$.

The main result of this section (Theorem XI.41) is that all of the above conjectures are correct. Recall that the Rollnik class R is the set of measurable functions $V(x)$ satisfying

$$\|V\|_R^2 = \int_{\mathbb{R}^6} \frac{|V(x)|\,|V(y)|}{|x-y|^2}\, dx\, dy < \infty$$

Theorem XI.41 Let V be in $R \cap L^1(\mathbb{R}^3)$. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and let $H = H_0 + V$ in the sense of quadratic forms (Theorem X.19). Then, there is a set $\mathscr{E} \subset \mathbb{R}_+$, the positive reals, which is closed, of Lebesgue measure zero, and such that:

(a) If $k^2 \notin \mathscr{E}$, then there is a unique solution $\varphi(\cdot, \mathbf{k})$ of the Lippmann–Schwinger equation (81) which obeys $|V|^{1/2}\varphi(\cdot, \mathbf{k}) \in L^2$.

(b) If $f \in L^2$, then

$$f^*(\mathbf{k}) = \text{l.i.m.}(2\pi)^{-3/2} \int \overline{\varphi(\mathbf{x}, \mathbf{k})} f(\mathbf{x})\, d\mathbf{x} \tag{82a}$$

exists.

(c) If $f \in D(H)$, then

$$(Hf)^*(\mathbf{k}) = k^2 f^*(\mathbf{k}) \tag{82b}$$

(d) $\text{Ran } ^* = L^2(\mathbb{R}^3)$ and (82c)

$$\int |f^*(\mathbf{k})|^2\, d\mathbf{k} = \|P_{ac}(H)f\|^2 \tag{82e}$$

More generally, if $[\alpha, \beta] \cap \mathscr{E}$ is empty and $\alpha > 0$, then

$$\int_{\alpha \le k^2 \le \beta} |f^*(\mathbf{k})|^2\, dk = \|P_{[\alpha,\beta]}(H)f\|^2 \tag{82e'}$$

where $\{P_\Omega(H)\}$ is the spectral family for H.

(e) Let L.I.M. stand for the L^2-limit as $M \to \infty$ and $\delta \to 0$ of the integral over $\{\mathbf{k} | k \le M, \text{dist}(k^2, \mathscr{E}) > \delta\}$. Then

$$(P_{ac}(H)f)(x) = \text{L.I.M.}(2\pi)^{-3/2} \int f^*(\mathbf{k})\varphi(\mathbf{x}, \mathbf{k})\, d\mathbf{k} \tag{82d}$$

(f) For any $f \in L^2$,

$$(\Omega^+ f)^*(\mathbf{k}) = \hat{f}(\mathbf{k}) \tag{83}$$

We shall sketch the major ideas in the proof of Theorem XI.41. The details may be found in the references in the Notes. But first we examine several consequences of the theorem and its proof. Notice first that (82e′) implies that for any interval $[\alpha, \beta]$, disjoint from $\mathscr{E}$ with $\alpha > 0$, Ran $P_{[\alpha,\beta]} \subset \mathscr{H}_{ac}$; so if any singular continuous spectrum exists, it must be in $\mathscr{E}$ since $\sigma_{ess}(H) = [0, \infty)$ by Theorem XIII.15. This will allow us to conclude that $\sigma_{sing}(H) = \varnothing$ in some cases (see Theorem XIII.21). Secondly, in the proof of Theorem XI.41, one uses the fact that Ω^+ exists but not its completeness. (83) says that $\#[\text{Ran } \Omega^+] = L^2$ and (82d) says that $\#^{-1}[L^2] = \mathscr{H}_{ac}$, so that Theorem XI.41 implies that Ran $\Omega^+ = \mathscr{H}_{ac}$. Thus, in case $V \in L^1 \cap R$, we have a proof of the completeness of $\Omega^\pm$ which does not use the Kato–Birman theory. In the Notes we explain how the eigenfunction expansion helps to "explain" the convergence of the wave operators when $V_n \to V$ in R and L^1. In the Notes we shall also discuss how the method used to prove Theorem XI.41 can be used to prove a similar result when $V \in L^p \cap L^{3/2}$ for some $1 \le p < \frac{3}{2}$ (see also Problem 57). We shall discuss similar eigenfunction expansions in a more general setting in the appendix and in the Notes. We also remark that if $\sigma_{sing}(H) = \varnothing$ (see Sections XIII.6, 7, 8), we can find a family $\{\varphi_n\}_{n=1}^N$ of square integrable eigenfunctions for H with $H\varphi_n = E_n\varphi_n$ so that, if $f_n^* = (\varphi_n, f)$, then

$$f(\mathbf{x}) = \text{L.I.M.}\left(\sum_{n=1}^{N} f_n^* \varphi_n(\mathbf{x}) + \int (2\pi)^{-3/2} \varphi(\mathbf{x}, \mathbf{k}) f^*(\mathbf{k})\, d\mathbf{k}\right)$$

$$\|f\|^2 = \sum_{n=1}^{N} |f_n^*|^2 + \int |f^*(\mathbf{k})|^2\, d\mathbf{k}$$

$$(Hf)^*(\mathbf{k}) = k^2 f^*(\mathbf{k}); \quad (Hf)_n^* = E_n f_n^*$$

We now turn to the main ideas in the proof of Theorem XI.41:

(I) *Modified Lippmann–Schwinger equation* We first introduce a modified Lippmann–Schwinger equation. If $\psi(x, k) = |V(x)|^{1/2}\varphi(x, k)$ and φ obeys (81), then ψ obeys

$$\psi(x, k) = |V(x)|^{1/2} e^{ik\cdot x} - \frac{1}{4\pi} \int \frac{|V(x)|^{1/2} e^{i|k||x-y|} V^{1/2}(y)}{|x-y|} \psi(y, k)\, dy \tag{84}$$

where $V^{1/2} = |V|^{1/2}(\text{sgn } V)$.

We first show that (84) has solutions. Since $V \in L^1 \cap R$, $e^{ik\cdot x}|V|^{1/2}$ is in $L^2(\mathbb{R}^3)$ and

$$\frac{|V(x)|^{1/2} e^{i|k||x-y|} V^{1/2}(y)}{|x-y|} \in L^2(\mathbb{R}^6)$$

for any k in $\mathbb{R}^3$. Thus the modified Lippmann–Schwinger equation has the form $\psi = \eta + L_{|k|}\psi$ where η is in L^2 and $L_{|k|}$ is a Hilbert–Schmidt operator. Let $\mathscr{E}$ be the set of $|k|^2 \in \mathbb{R}_+$ such that the homogeneous equation $\psi = L_{|k|}\psi$ has a nonzero solution in L^2. By the Fredholm alternative (corollary to Theorem VI.14), (84) has a unique L^2 solution ψ whenever $|k|^2 \notin \mathscr{E}$. It follows that the original Lippmann–Schwinger equation has a unique solution φ satisfying $|V|^{1/2}\varphi \in L^2(\mathbb{R}^3)$ given by

$$\varphi(x, k) = e^{ik\cdot x} - \frac{1}{4\pi} \int \frac{e^{i|k||x-y|}}{|x-y|} V^{1/2}(y)\psi(y, k)\, dy$$

Of course, one must do a little arguing to show this last integral converges a.e. in x, but we are not giving the details of such subtleties in this sketch.

(II) *Study of the set $\mathscr{E}$* Let K_λ be the operator $|V|^{1/2}(H_0 - \lambda^2)^{-1}V^{1/2}$. This is the integral operator (84) when $\lambda = |k|$ for some $k \in \mathbb{R}^3$, in particular, for real positive λ. K_λ is easily shown to be analytic when Im $\lambda > 0$ and continuous when Im $\lambda \ge 0$. Moreover, by the dominated convergence theorem, one can show that the Hilbert–Schmidt norm of K_λ goes to 0 as Im $\lambda \to \infty$. Thus $(I + K_\lambda)^{-1}$ exists as long as Im λ is large. At this point we need a slight improvement of the analytic Fredholm theorem (Theorem VI.14), namely:

Proposition Let $A(\lambda)$ be a compact operator-valued function in $\mathcal{D} = \{\lambda | \text{Im } \lambda \ge 0\}$ which is continuous in D and analytic in its interior. Then either $(1 - A(\lambda))^{-1}$ exists for no λ in D or $\{\lambda | \text{Im } \lambda = 0$, and $(1 - A(\lambda))^{-1}$ does not exist$\}$ is a closed subset of $\mathbb{R}$ with measure 0.

This proposition follows from the method of proof of Theorem VI.14 together with a fact about analytic functions: The real zeros of a function analytic in the open upper half-plane and continuous in the closed half-plane is a closed subset of $\mathbb{R}$ of measure 0 (see Problems 58 and 59 and the Notes). Thus the subset $\mathscr{E} \subset \mathbb{R}$ defined in part I is closed with measure 0.

We make several remarks about $\mathscr{E}$: First, $\mathscr{E}$ is always bounded. This follows from the fact that the operator norm of K_λ goes to zero as $\lambda \to \infty$, λ real, due to the oscillations of the kernel. These oscillations are controlled by the Riemann–Lebesgue lemma (Problem 60). Secondly, we note that there

are two cases in which we have control on $\mathscr{E}$. If $\|V\|_R < 4\pi$, then $\|K_\lambda\| < 1$ for all λ so $\mathscr{E} = \varnothing$. Or, if V falls off exponentially in the sense that $e^{\alpha|x|}V(x) \in R$ for some $\alpha > 0$, then $\mathscr{E}$ is finite. This is because in that case K_λ can be continued to the region $\{\lambda \mid \operatorname{Im}\lambda > -\alpha/2\}$ so that the ordinary analytic Fredholm theorem implies that $\mathscr{E}$ is discrete.

(III) *Study of the Green's function* The basic idea of the proof is to relate the functions $\varphi(x, k)$ to the integral operator $(H - E)^{-1}$ and then to relate $(H - E)^{-1}$ to the spectral projections via Stone's formula (Theorem VII.13),

$$\operatorname*{s-lim}_{\varepsilon \downarrow 0} (2\pi i)^{-1} \int_\alpha^\beta [(H - \mu - i\varepsilon)^{-1} - (H - \mu + i\varepsilon)^{-1}]\, d\mu = \tfrac{1}{2}P_{(\alpha,\beta)} + \tfrac{1}{2}P_{[\alpha,\beta]}$$

As a preliminary, it is necessary to study the integral kernel of $(H - E)^{-1}$.

Lemma 1 Suppose $E \notin \sigma(H)$. Then there exists a measurable function $G(x, y; E)$ on $\mathbb{R}^3 \times \mathbb{R}^3$, so that

$$[(H - E)^{-1}\psi](x) = \int G(x, y; E)\psi(y)\, dy$$

Moreover:

(a) For almost every fixed x, $G(x, \cdot; E) \in L^1 \cap L^2$.
(b) $G(x, y; E) = G(y, x; E)$ and $\overline{G(x, y; E)} = G(x, y; \bar{E})$.
(c) G obeys the integral equation

$$G(x, y; E) = G_0(x, y; E) - \int G_0(x, z; E)V(z)G(z, y; E)\, dz$$

where $G_0(x, y; E) = e^{i\sqrt{E}|x-y|}/4\pi|x - y|$ is the free Green's function where we take the value of $\sqrt{E}$ with the positive imaginary part.

Proof We present the formal elements of the proof, not worrying about convergence of integrals or domain questions. By a simple argument (Problem 61),

$$(H - E)^{-1} = (H_0 - E)^{-1} - [(H_0 - E)^{-1}V^{1/2}] \times [1 + |V|^{1/2}(H_0 - E)^{-1}V^{1/2}]^{-1}[|V|^{1/2}(H_0 - E)^{-1}]$$

Since $V \in L^1$, the kernel $|V(x)|^{1/2}e^{i\sqrt{E}|x-y|}/4\pi|x - y|$ of $|V|^{1/2}(H_0 - E)^{-1}$ is Hilbert–Schmidt. Thus $(H - E)^{-1} - (H_0 - E)^{-1}$ is Hilbert–Schmidt and so is an integral operator with a square integrable kernel $A(x, y)$. In particular, $A(x, \cdot) \in L^2$ for almost every x. Since $(H_0 - E)^{-1}$ has integral kernel G_0 with $G_0(x, \cdot) \in L^2$ for almost all x, $(H - E)^{-1}$ has an integral kernel with

$G(x, \cdot; E) \in L^2$ a.e. in x. The integral equation (c) is just a translation of $(H - E)^{-1} = (H_0 - E)^{-1} - (H_0 - E)^{-1}V(H - E)^{-1}$. In particular, if Re E is sufficiently negative, the integral equation can be solved by iteration. For such E, (b) follows from the analogous properties of G_0 and the fact that V is real. Thus (b) holds for all $E \notin \sigma(H)$ by analytic continuation. It remains to show that $G(x, \cdot; E) \in L^1$ a.e. in x. This can be done by using the integral equation (Problem 61b). ∎

G is called the **Green's function** for H.

(IV) *Positive eigenvalues* As another preliminary, we need the fact:

Lemma 2 If $E > 0$ and $E \notin \mathscr{E}$, then E is not an eigenvalue of H.

This is left to the reader (Problem 62 or see the reference in the Notes). It implies that whenever $[\alpha, \beta] \cap \mathscr{E} = \varnothing$, $P_{[\alpha,\beta]} = P_{(\alpha,\beta)}$ so that the term $\frac{1}{2}[P_{[\alpha,\beta]} + P_{(\alpha,\beta)}]$ in Stone's formula is $P_{(\alpha,\beta)} = P_{[\alpha,\beta]}$.

(V) *The relation of # and the resolvent* Suppose Im $\kappa > 0$ and Re $\kappa \neq 0$. Since $G(x, \cdot; \kappa^2) \in L^1$, it has an inverse Fourier transform $g(x, k; \kappa) \equiv (2\pi)^{-3/2} \int G(x, y; \kappa^2)e^{ik\cdot y}\, d^3y$ which is continuous. Define $h(x, k; \kappa) \equiv (2\pi)^{3/2}(|k|^2 - \kappa^2)g(x, k; \kappa)$. Then the integral equation for G translates into an integral equation for h (after a side argument which allows the interchange of the Fourier transform integral and the integral equation integral):

$$h(x, k; \kappa) = e^{ik\cdot x} - \frac{1}{4\pi}\int \frac{e^{i\kappa|x-y|}}{|x - y|} V^{1/2}(y)p(y, k; \kappa)\, dy \tag{85a}$$

$$p(y, k; \kappa) = |V(y)|^{1/2}e^{ik\cdot y} - \frac{1}{4\pi}\int |V(y)|^{1/2} \frac{e^{i\kappa|x-y|}}{|x - y|} V^{1/2}(x)p(x, k; \kappa)\, dx \tag{85b}$$

The key fact is the relation between (85b) and the modified Lippmann–Schwinger equation (84). If $k \in \mathbb{R}^3$ is fixed and $\kappa = |k|$, the equation for $p(\cdot, k; \kappa)$ becomes identical to the equation for $\psi(\cdot, k)$. This can be used to prove:

Lemma 3 Let $f \in C_0^\infty(\mathbb{R}^3)$. Then the integrals

$$\Phi(k; \kappa) = (2\pi)^{-3/2} \int \overline{h(x, k; \kappa)} f(x)\, d^3x$$

and

$$f^*(k) = (2\pi)^{-3/2} \int \overline{\varphi(x, k)} f(x)\, d^3x$$

converge absolutely if $\operatorname{Im} \kappa > 0$ in the Φ integral or if $|k|^2 \notin \mathscr{E}$ in the f^* integral. Suppose that $[\alpha, \beta] \cap \mathscr{E} = \varnothing$ with $\alpha > 0$. Then $\Phi(k; \kappa)$ has an extension to the region $\alpha^{1/2} \le \operatorname{Re} \kappa \le \beta^{1/2}$, $\operatorname{Im} \kappa \ge 0$, which is uniformly continuous in k and κ, and for $k^2 \in [\alpha, \beta]$

$$f^*(k) = \Phi(k;\ |k|)$$

We thus have related f^* to the boundary value of the resolvent.

(VI) *Proof of (82e') when $f \in C_0^\infty$:*

Lemma 4 Let $f \in C_0^\infty$ and let $[\alpha, \beta] \cap \mathscr{E} = \varnothing$ with $\alpha > 0$. Then

$$\|P_{[\alpha, \beta]} f\|^2 = \int_{\alpha^{1/2} < |k| < \beta^{1/2}} |f^*(k)|^2\, d^3k$$

Proof Again, we shall not provide the technical details. Let $\kappa^2 = \mu + i\varepsilon$ with $\varepsilon > 0$, and $\operatorname{Im} \kappa > 0$. Up to a factor of $(2\pi)^{3/2}(|k|^2 - \mu - i\varepsilon)$, $h(x, \cdot; \kappa)$ is the Fourier transform of $G(x, \cdot; \kappa^2)$ so the Plancherel theorem implies that

$$(\kappa^2 - \bar\kappa^2) \int \overline{G(z, x; \bar\kappa^2)} G(z, y, \bar\kappa^2)\, dz$$

$$= \int \frac{2i\varepsilon}{(k^2 - \mu)^2 + \varepsilon^2} h(x, k; \kappa) \overline{h(y, k; \kappa)}\, \frac{dk}{(2\pi)^3} \tag{86}$$

If we multiply the left-hand side of (86) by $\overline{f(x)} f(y)$ and integrate, we obtain

$$(\kappa^2 - \bar\kappa^2)(R_{\bar\kappa^2} f, R_{\bar\kappa^2} f) = (\kappa^2 - \bar\kappa^2)(f, R_{\kappa^2} R_{\bar\kappa^2} f) = (f, R_{\kappa^2} - R_{\bar\kappa^2} f)$$

where $R_E \equiv (H - E)^{-1}$. On the other hand, the right-hand side of (86) then becomes

$$\int \frac{2i\varepsilon}{(|k|^2 - \mu)^2 + \varepsilon^2} |\Phi(k; \sqrt{\mu + i\varepsilon})|^2\, dk$$

We thus conclude that

$$\int_\alpha^\beta (f, [R_{\mu + i\varepsilon} - R_{\mu - i\varepsilon}] f) \frac{d\mu}{2\pi i} = \frac{1}{\pi} \int_\alpha^\beta \int \frac{\varepsilon}{(|k|^2 - \mu)^2 + \varepsilon^2} |\Phi(k, \sqrt{\mu + i\varepsilon})|^2\, d\mu\, dk \tag{87}$$

As $\varepsilon \to 0$, Stone's formula and Lemma 2 imply that the left-hand side of (87) approaches $(f, P_{[\alpha, \beta]} f) = \|P_{[\alpha, \beta]} f\|^2$. Formally, $\varepsilon\pi^{-1}[(|k|^2 - \mu)^2 + \varepsilon^2]^{-1}$ approaches $\delta(k^2 - |\mu|)$ as $\varepsilon \to 0$ (see (V.4)), so that one can show that the right side of (87) approaches $\int_{\alpha < |k^2| < \beta} |f^*(k)|^2\, dk$ by using Lemma 3. ∎

(VII) *Extension to general f* Using Lemma 4, polarization, and a variety of limiting arguments, it is now easy to prove the remainder of Theorem XI.41 with the three exceptions: (i) Ran $\# = L^2$, (ii) $(\Omega^+ f)^* = \hat f$, and (iii) equation (82b). At this stage the formula (82b) is only proven in weak form. Once it is proven that Ran $\# = L^2$, we then get (82b). For details, see the reference in the Notes.

(VIII) *Reduction to (88)* Suppose that we can prove

$$\widehat{((\Omega^+)^* f)} = f^* \tag{88}$$

Then (83) follows from

$$(\Omega^+ f)^* = \widehat{(\Omega^+)^* \Omega^+ f} = \hat f$$

and Ran $\# = L^2$ follows from the fact that $\hat{}$ and $(\Omega^+)^*$ are surjective. Thus proving (88) completes the proof of Theorem XI.41.

(IX) *Aside on abelian limits* To prove (88) we need the following:

Lemma 5 Let $f(x)$ be a bounded measurable function and suppose that $\lim_{t \to \infty} \int_0^t f(x)\, dx = a$. Then $\lim_{\varepsilon \downarrow 0} \int_0^\infty e^{-\varepsilon s} f(s)\, ds = a$.

Proof Let $g(t) = \int_0^t f(s)\, ds$ and $q(\varepsilon) = \int_0^\infty e^{-\varepsilon s} f(s)\, ds$. Then $g'(t) = f(t)$ a.e., so an integration by parts proves that

$$q(\varepsilon) = \int_0^\infty \varepsilon e^{-\varepsilon s} g(s)\, ds$$

Using the facts that g is bounded, $g(t) \to a$ as $t \to \infty$, and $\int_0^\infty \varepsilon e^{-\varepsilon s}\, ds = 1$, it is easy to prove that $q(\varepsilon) \to a$ (Problem 63). ∎

(X) *Conclusion* We are ready to conclude our sketch of the proof of Theorem XI.41.

Proof of (88) We need only prove the result for $f \in \mathscr{H}_{ac}$, the absolutely continuous space for H. For, if $f \in \mathscr{H}_{ac}^{\perp}$, then $(\Omega^+)^* f = 0$ and, by (82e) proven in VII, $f^* = 0$. Thus it is sufficient to prove that

$$(f, \Omega^+ g) = \int \overline{f^*(k)} \hat{g}(k)\, dk \tag{89}$$

for a set of g dense in $\mathscr{H}$ and a set of f dense in $\mathscr{H}_{ac}$. We shall suppose that f^* has support in some interval $[\alpha, \beta]$ disjoint from $\mathscr{E}$ and that $g \in C_0^\infty$. In the computations below we shall not use these technical assumptions on f and g explicitly, but we shall interchange limits and multiple integrals; in justifying these interchanges the technical assumptions on f and g are useful.

Since $f, g \in Q(H) = Q(H_0)$, by Problem 20,

$$(f, \Omega^+ g) - (f, g) = i \lim_{t \to -\infty} \int_0^t (f, e^{iHs} V e^{-iH_0 s} g)\, ds$$

Thus, by Lemma 5,

$$(f, \Omega^+ g) = (f, g) + i \lim_{\varepsilon \downarrow 0} \int_0^{-\infty} (f, e^{iHt} V e^{-iH_0 t} g) e^{\varepsilon t}\, dt \tag{90}$$

From (82e'), it is easy to prove that $(f, e^{iHt} g) = \int \overline{f^*(k)} e^{ik^2 t} g^*(k)\, dk$ if either f or g is in $\mathscr{H}_{ac}$. As a result

$$(f, e^{iHt} V e^{-iH_0 t} g) = \int \overline{f^*(k)} e^{ik^2 t} (V e^{-iH_0 t} g)^*(k)\, dk$$

$$= (2\pi)^{-3/2} \iint \overline{f^*(k)} e^{ik^2 t} \overline{\varphi(x, k)} V(x) (e^{-iH_0 t} g)(x)\, dx\, dk$$

Thus

$$\int_0^{-\infty} (f, e^{iHt} V e^{-iH_0 t} g) e^{\varepsilon t}\, dt$$

$$= (2\pi)^{-3/2} \int_0^{-\infty} \iint \overline{f^*(k) \varphi(x, k)} V(k) (e^{-it(H_0 - k^2 + i\varepsilon)} g)(x)\, dx\, dk\, dt$$

$$= -i(2\pi)^{-3/2} \iint \overline{f^*(k) \varphi(x, k)} V(x) [(H_0 - k^2 + i\varepsilon)^{-1} g](x)\, dx\, dk$$

$$= \frac{-i}{4\pi} (2\pi)^{-3/2} \iiint \overline{f^*(k) \varphi(x, k)} V(x) \frac{e^{-i|x-y|\sqrt{k^2 - i\varepsilon}}}{|x - y|} g(y)\, dx\, dy\, dk$$

Taking $\lim_{\varepsilon \downarrow 0}$ inside the integral in (90), we see that

$$(f, \Omega^+ g) = (f, g) + (2\pi)^{-3/2} \iint \overline{f^*(k)} g(y)$$

$$\times \left[\frac{1}{4\pi} \int \frac{e^{-ik|x-y|}}{|x - y|} V(x) \overline{\varphi(x, k)}\, dx \right] dk\, dy$$

$$= (f, g) + (2\pi)^{-3/2} \int \overline{f^*(k)} g(y) [e^{-ik \cdot y} - \overline{\varphi(y, k)}]\, dk\, dy$$

$$= (f, g) + \int \overline{f^*(k)} \hat{g}(k)\, dk - \int \overline{f^*(k)} g^*(k)\, dk$$

$$= \int \overline{f^*(k)} \hat{g}(k)\, dk$$

In the second line above we used the Lippmann–Schwinger equation and at the last step we used (82e). This completes the proof of (89) and so of (88). Our sketch of the proof of Theorem XI.41 is thus concluded. ∎

The Lippmann–Schwinger eigenfunctions $\varphi(x, k)$ are especially useful because they can be used to express the S-matrix. First, we introduce an auxiliary object:

Definition Let $\mathbf{k} \in \mathbb{R}^3$, $\mathbf{k}' \in \mathbb{R}^3$, $k'^2 \notin \mathscr{E}$. Define

$$T(\mathbf{k}, \mathbf{k}') = (2\pi)^{-3} \int e^{-i\mathbf{k} \cdot \mathbf{x}} V(\mathbf{x}) \varphi(\mathbf{x}, \mathbf{k}')\, d\mathbf{x}$$

$T(\cdot, \cdot)$ is called the ***T*-matrix.**

Theorem XI.42 $T(\mathbf{k}, \mathbf{k}')$ is uniformly continuous in any region of the form $\mathbb{R}^3 \times \{\mathbf{k}' \mid k'^2 \in [\alpha, \beta]\}$ where $\alpha > 0$ and $[\alpha, \beta] \cap \mathscr{E} = \varnothing$. Moreover, if $f, g \in \mathscr{S}(\mathbb{R}^3)$ where $\hat{f}$ and $\hat{g}$ are functions with supports in spherical shells disjoint from $\{\mathbf{k}' \mid k'^2 \in \mathscr{E}\}$, then

$$(f, (S - I)g) = (-2\pi i) \int \overline{\hat{f}(\mathbf{k})} \hat{g}(\mathbf{k}') T(\mathbf{k}, \mathbf{k}')\, \delta(k^2 - (k')^2)\, d\mathbf{k}\, d\mathbf{k}' \tag{91}$$

Before proving Theorem XI.42, we make a series of remarks. First, the $\delta(k^2 - (k')^2)$ in (91) is a shorthand way of writing

$$\int \overline{\hat{f}(\mathbf{k})} \left[\int_{k'^2 = k^2} T(\mathbf{k}, \mathbf{k}') \hat{g}(\mathbf{k}') (\tfrac{1}{2} k')\, d\Omega(\mathbf{k}') \right] d\mathbf{k}$$

where $d\Omega(\mathbf{k}')$ is the angular measure on the sphere and $\frac{1}{2}k'$ is the Jacobian of the coordinate change from $\mathbf{k}'$ to $\langle (k')^2, \Omega(\mathbf{k}')\rangle$. (91) is often written symbolically as

$$S(\mathbf{k}, \mathbf{k}') = \delta(k - k') - 2\pi i T(\mathbf{k}, \mathbf{k}')\, \delta(k^2 - (k')^2)$$

This is a realization of the scheme discussed at the end of Section 5.

We also note that the set of f and g allowed in (91) is dense in L^2, so that φ completely determines S. Notice that S is completely determined by the values of $T(\mathbf{k}, \mathbf{k}')$ when $k = k'$. This set of values is known as the "on-shell T-matrix" or as the T-matrix "on the energy shell." It is a typical occurrence in physical theories, and in particular occurs in perturbation theoretic quantum field theory, that scattering is described in terms of an "on-shell" quantity which the theory also determines "off-shell." One of the beauties of Faddeev's three-body theory is that the *off-shell* T-matrix for the two-body system enters the theory of three-body scattering. We shall not have a chance to discuss this further.

Proof of Theorem XI.42 Since $S = (\Omega^-)^*\Omega^+$ and $I = (\Omega^+)^*\Omega^+$,

$$\begin{aligned}
(f, (S - I)g) &= (f, (\Omega^- - \Omega^+)^*\Omega^+ g) \\
&= ((\Omega^- - \Omega^+)f, \Omega^+ g) \\
&= \lim_{T\to\infty} \int_{-T}^{T} (e^{iHt}(iV)e^{-iH_0t}f, \Omega^+ g)\, dt \\
&= \lim_{\varepsilon \downarrow 0} (-i) \int_{-\infty}^{\infty} e^{-\varepsilon|t|} (e^{iHt} V e^{-iH_0t} f, \Omega^+ g)\, dt \\
&= \lim_{\varepsilon \downarrow 0} (-i) \int_{-\infty}^{\infty} e^{-\varepsilon|t|} \\
&\quad \times \left(\int \overline{[e^{iHt} V e^{-iH_0t} f]}^*(k') [\Omega^+ g]^*(k')\, dk' \right) dt \qquad (92)
\end{aligned}$$

In the next to the last step we used Lemma 5, and in the last step we have used (82e) of Theorem XI.41 and the fact that $\Omega^+ g \in \mathscr{H}_{ac}$. By (83),

$$(\Omega^+ g)^*(k') = \hat{g}(k')$$

and by (82),

$$\begin{aligned}
[e^{iHt} V e^{-iH_0t} f]^*(k') &= e^{i|k'|^2 t} [V e^{-iH_0t} f]^*(k') \\
&= (2\pi)^{-3/2} \int e^{i|k'|^2 t} V(x) (e^{-iH_0t} f)(x) \overline{\varphi(x, k')}\, dx \\
&= (2\pi)^{-3} \int e^{i[|k'|^2 - |k|^2]t} V(x) e^{ik\cdot x} \overline{\varphi(x, k')} \hat{f}(k)\, dx\, dk
\end{aligned}$$

Thus the expression in (92) is

$$(-i)(2\pi)^{-3} \int_{-\infty}^{\infty} dt \left[\int e^{i(|k|^2 - |k'|^2)t - \varepsilon|t|} V(x) \varphi(x, k') e^{-ik\cdot x} \overline{\hat{f}(k)} \hat{g}(k')\, dk'\, dx\, dk \right]$$

Doing the t-integration,

$$(f, (S - I)g) = \lim_{\varepsilon \downarrow 0} \int (-i) T(k, k') \frac{2\varepsilon}{(|k|^2 - |k'|^2)^2 + \varepsilon^2} \overline{\hat{f}(k)} \hat{g}(k')\, dk\, dk' \qquad (93)$$

By definition, $T(k, k')$ is the inner product of $f_k(x) = (2\pi)^{-3} e^{-ik\cdot x} V^{1/2}(x)$ and $\psi(x, k')$. Since $\psi(\cdot, k')$ is uniformly L^2-continuous in the regions considered and $f_k(\cdot)$ is uniformly L^2-continuous since $V \in L^1$, $T(k, k')$ has the claimed continuity properties. As a result, the formula, $2\varepsilon[(|k|^2 - |k'|^2) + \varepsilon^2]^{-1} \to 2\pi\, \delta(|k|^2 - |k'|^2)$ valid as measures on $\kappa(\mathbb{R}^6)$ can be applied to (93). This completes the proof of (91). ∎

There is an alternative proof to this theorem in certain circumstances; see the third appendix to Section 8 or Problem 67.

Now that we have the connection between the eigenfunctions and S, we can develop the theory in various directions. Since φ obeys the Lippmann–Schwinger equation (81), there is a formal series for φ by iteration and thus a series for T:

$$T(\mathbf{k}, \mathbf{k}') = \sum_{n=0}^{\infty} T_n(\mathbf{k}, \mathbf{k}') \qquad (94a)$$

$$T_0(\mathbf{k}, \mathbf{k}') = (2\pi)^{-3} \int e^{i(\mathbf{k}' - \mathbf{k})\cdot \mathbf{x}} V(x)\, dx \qquad (94b)$$

$$\begin{aligned}
T_n(k, k') &= (2\pi)^{-3} (-1)^n (4\pi)^{-n} \int e^{-i\mathbf{k}\cdot \mathbf{x}_0} V(\mathbf{x}_0) \\
&\quad \times \frac{e^{ik'|\mathbf{x}_0 - \mathbf{x}_1|}}{|\mathbf{x}_0 - \mathbf{x}_1|} V(\mathbf{x}_1) \frac{e^{ik'|\mathbf{x}_1 - \mathbf{x}_2|}}{|\mathbf{x}_1 - \mathbf{x}_2|} V(\mathbf{x}_2) \\
&\quad \cdots V(\mathbf{x}_{n-1}) \frac{e^{ik'|\mathbf{x}_{n-1} - \mathbf{x}_n|}}{|\mathbf{x}_{n-1} - \mathbf{x}_n|} V(\mathbf{x}_n) e^{ik'\cdot \mathbf{x}_n}\, dx_0 \cdots dx_n
\end{aligned}$$

The series (94b) is called the **Born series** for T and the leading term (94b) is called the **Born amplitude**. Because of our study of $\mathscr{E}$ ((II) in the sketch of the proof of Theorem XI.41; see also Problem 60), we can easily prove that in certain cases the Born series converges.

Theorem XI.43 Let $V \in L^1 \cap R$.

(a) There exists a number K so that the Born series for $T(\mathbf{k}, \mathbf{k}')$ converges if $(k')^2 > K^2$, $\mathbf{k} \in \mathbb{R}^3$.

(b) If $\|V\|_R^2 < 4\pi$, then the Born series for $T(\mathbf{k}, \mathbf{k}')$ converges for all $\mathbf{k}$, $\mathbf{k}' \in \mathbb{R}^3$.

Proof $T(k, k')$ is the inner product of a fixed L^2-vector with the modified Lippmann–Schwinger function $\psi(x, k') = |V(x)|^{1/2}\varphi(x, k')$. ψ obeys an L^2 integral equation whose iteration leads to the Born series. If the series for ψ converges in L^2 for some k', then the Born series converges for that value of k' and all k. To show that the series for ψ converges, it is enough to show that the kernel of the integral equation it satisfies is the kernel of an integral operator $K_{k'}$ with norm less than 1. For $V \in R$, we know that $\lim_{k' \to \infty} \|K_{k'}\| = 0$ (Problem 60), so (a) holds. If $\|V\|_R^2 < 4\pi$, then $\|K_{k'}\|_{\text{H.S.}} = (4\pi)^{-1/2}\|V\|_R < 1$ for all k'. ∎

Using the methods of Section 7, it can be shown that if $V \in R$ and if $S(\lambda)$ is the S-operator for $-\Delta + \lambda V$, λ real, then $S(\lambda)$ has an operator-valued analytic continuation to the region $\{\lambda \mid |\lambda|\, \|V\|_R < 4\pi\}$. Theorem XI.43 is just one of many results about recovering S from a Born series or from some other formal series. Using the Fredholm theory for solving L^2 equations with Hilbert–Schmidt kernels, one can find convergent series $N(\mathbf{k}, \mathbf{k}')$ and $D(k')$ with $D(\alpha) \neq 0$ if $\alpha^2 \notin \mathscr{E}$ so that $T(\mathbf{k}, \mathbf{k}') = N(\mathbf{k}, \mathbf{k}')/D(k')$. This realization of T is the start of an analysis of the convergence of the Padé approximants formed from the Born series. This summability method can be shown to converge in some cases where the Born series diverges (see the Notes). In addition, there are a variety of results concerning convergence of series for the "partial wave amplitudes" discussed in Section 8.

A second consequence of the relation between T and S is the *unitarity relation for* T, (95).

Theorem XI.44 Let $V \in L^1 \cap R$ and suppose that $\alpha^2 \notin \mathscr{E}$. Then for any $\mathbf{k}, \mathbf{k}' \in R^3$ with $k = k' = \alpha$,

$$\text{Im } T(k, k') = \pi \int \overline{T(k'', k)} T(k'', k')\, \delta((k'')^2 - \alpha)\, d^3k'' \tag{95}$$

Proof Since $\mathscr{E}$ is closed, we can find β, γ with $\alpha \in (\beta, \gamma)$ and $[\beta^2, \gamma^2] \cap \mathscr{E} = \varnothing$. By Theorem XI.42, if f is in $\mathscr{S}$ and $\hat{f}$ has support in $F = \{\mathbf{k} \mid \beta < k < \gamma\}$, then $\widehat{(Sf)}(k) = \hat{f}(k) - (2\pi i) \int T(k, k')\hat{f}(k')\, \delta(k^2 - k'^2)\, dk'$. By a simple limiting argument, this formula holds if $\hat{f}$ is merely continuous (with

support in F) and the map $M: \hat{f} \mapsto \widehat{Sf}$ takes the continuous functions with support in F into themselves. The adjoint of M is clearly given by

$$(M^*g)(k) = g(k) + (2\pi i) \int \overline{T(k', k)} g(k')\, \delta(k^2 - k'^2)\, dk'$$

The relation $M^*M = 1$, which follows from $S^*S = I$, implies that for almost all pairs $\langle k, k' \rangle$ with $|k| = |k'|$ and $k, k' \in F$, (95) holds. Since both sides are continuous in $\langle k, k' \rangle$ in the region $\{\langle k, k' \rangle \in F \times F \mid |k| = |k'|\}$, (95) holds throughout the region. ∎

To understand the importance of the unitarity relation for T, we must understand what quantity is measured in a scattering experiment. For simplicity, we suppose that V is spherically symmetric so that $T(\mathbf{k}, \mathbf{k}')$ depends only on k, k' and $\mathbf{k} \cdot \mathbf{k}'$. Given k and $\cos\theta \in [-1, 1]$, find $\mathbf{k}$, $\mathbf{k}'$ with $k' = k$ and $\mathbf{k} \cdot \mathbf{k}' = k^2 \cos\theta$. Then, the **scattering amplitude** $f(k, \theta)$ is defined by

$$f(k, \theta) \equiv -2\pi^2 T(\mathbf{k}, \mathbf{k}') \tag{96}$$

An argument which is partially heuristic and which we summarize in the Notes shows that if one sends in a beam of particles of energy $E = k^2$, the differential cross section (see Section 2) is given by

$$d\sigma/d\Omega = |f(k, \theta)|^2 \tag{97a}$$

The total cross section is thus given by

$$\sigma \equiv \int \frac{d\sigma}{d\Omega}\, d\Omega = 2\pi \int_{-\pi}^{\pi} |f(k, \theta)|^2 \sin\theta\, d\theta \tag{97b}$$

If we write the unitarity relation with $\mathbf{k} = \mathbf{k}'$, then it says

$$\text{Im } T(\mathbf{k}, \mathbf{k}) = \frac{\pi |\mathbf{k}|}{2} \int |T(\mathbf{k}'', \mathbf{k})|^2\, d\Omega(\mathbf{k}'')$$

or that

$$\sigma = \frac{4\pi}{k} \text{Im } f(k, 0) \tag{97c}$$

The relation (97c) is often called the **optical theorem**. Physically, it is an expression of the fact that the amount scattered out of the beam (the left-hand side of (97c)) must be compensated for by the interference between the original beam and the forward scattered wave (the right-hand side of (97c)).

We thus see that only the magnitude of f is directly measurable via (97a). Unitarity provides a partial handle for determining the argument of f. For

example, using (97c) one can determine $\arg f(k, 0)$ up to an ambiguity of reflection about the imaginary axis if one knows $(d\sigma/d\Omega)(k, \theta)$ for all θ. And, in fact, we saw in Section V.6 that if $d\sigma/d\Omega$ is sufficiently "small," then unitarity and the differential cross section determine f uniquely, for all θ.

Appendix to XI.6: Introduction to eigenfunction expansions by the auxiliary space method

In this section we developed eigenfunction expansions by solving a modified Lippmann–Schwinger equation in L^2. It is often useful to follow a somewhat different path which depends on a Banach space X which is continuously imbedded as a dense subspace $X \subset \mathscr{H}$. Under this situation we can naturally imbed $\mathscr{H}$ into X^* and thus X into X^* using the duality of $\mathscr{H}$; that is, for $\varphi \in \mathscr{H}$, define $\ell_\varphi \in X^*$ by $\ell_\varphi(x) = (\varphi, x)$. The triple $X \subset \mathscr{H} \subset X^*$ is reminiscent of the construction of $\mathscr{H}_1 \subset \mathscr{H} \subset \mathscr{H}_{-1}$ in the theory of quadratic forms (Theorem VIII.15).

Given the triple $X \subset \mathscr{H} \subset X^*$ one tries to obtain an eigenfunction expansion by a two-step process: (i) Show that $(H - z)^{-1}: X \to X^*$ extends continuously from $\operatorname{Im} z > 0$ to the real axis or the real axis with an exceptional set removed. (ii) Use the operators $(H - k^2 - i0)^{-1}$ to obtain generalized eigenfunctions $\varphi \in X^*$. (i) implies that $(f, (H - z)^{-1}f)$ has an extension to the real axis for $f \in X$; and, as we shall see in Section XIII.6, this implies that H has no singular continuous spectrum. For this reason, just developing step (i) is of considerable interest; we shall make just this kind of development in Section XIII.8 for a very large class of operators $-\Delta + V$ using rather subtle arguments. Here we want to illustrate the ideas of (i) by taking the extremely special situation where V falls off exponentially. We shall then describe step (ii) for the case where we are, in addition, in one dimension. The Notes give extensive references to the theory in more general circumstances.

Let X_a be the Hilbert space of functions with $e^{a|x|}f \in L^2 \equiv \mathscr{H}$ with the natural norm. Then for $a > 0$, $X_a \subset \mathscr{H} \subset X_{-a} = X_a^*$ as above. We first claim:

Lemma 1 The function $(-\Delta - k^2)^{-1}: X_a \to X_{-a}$, defined for $\operatorname{Im} k > 0$, extends analytically to the region $\operatorname{Im} k > -a$, $\arg k \neq -\frac{1}{2}\pi$, as an analytic function with values in the compact operators from X_a to X_{-a}. The same thing is true of the functions $\partial_i(-\Delta - k^2)^{-1}$.

Proof Let $G_0(x, y; E)$ be the integral kernel of $(-\Delta - E)^{-1}$ for $E \notin [0, \infty)$ defined uniquely for all x, y with $x \neq y$ by demanding continuity. We first claim that $G_0(x, y; E)$ extends analytically to all $\sqrt{E}$ with $\arg(\sqrt{E}) \neq -\frac{1}{2}\pi$ and obeys the estimate

$$|G_0(x, y; E)| \leq C_{\varepsilon,\delta}(|x - y|^{-(n-2)} + E^{(n-2)/2})e^{|x-y|(|\operatorname{Im}\sqrt{E}| + \varepsilon|E|^{1/2})} \tag{98}$$

if $n \geq 3$ and $(\operatorname{Re}\sqrt{E})/|\sqrt{E}| \geq \delta$. If $n = 1$, a similar estimate holds with no $|x - y|^{-(n-2)}$ term; and if $n = 2$, the term before the exponential is replaced by $|\ln(|x - y|^{-1}E^{1/2})| + 1$. (98) is obvious if $n = 3$ or $n = 1$ from the explicit form that G_0 takes. For general n, the proof of (98), which is *not* the best possible estimate, is left to the reader (Problem 65).

Let $H(x, y; k)$ be the function $e^{-a|x|}G_0(x, y; k^2)e^{-a|y|}$. By (98), for any k with $\operatorname{Im} k > -a$, $\arg k \neq -\frac{1}{2}\pi$,

$$|H(x, y; k)| \leq h_k(x - y)$$

with $h_k \in L^1$. For $n \geq 3$, $h_k(x) = \text{const}\ |x - y|^{-(n-2)}e^{-\gamma|x|}$; for $n = 2$, $h_k(x) = \text{const}\ (|\ln|x|| + 1)e^{-\gamma|x|}$; and, for $n = 1$, $h_k(x) = \text{const}\ e^{-\gamma|x|}$. It follows by Young's inequality that $H(x, y; k)$ is the kernel of a bounded integral operator. The operator is clearly analytic in k and, by Theorem IX.20, it is compact for $\operatorname{Im} k > 0$ and so for all k by analytic continuation and the fact that the compact operators are norm closed. Thus, $e^{-a|x|}(-\Delta - k^2)^{-1}e^{-a|y|}$ is an analytic function with values in the compact operators on L^2 for $\operatorname{Im} k > -a$, $\arg k \neq -\pi$. Since $e^{\pm a|x|}$ is a unitary map from L^2 to $X_{\mp a}$, the result is proven. The $\partial_i(-\Delta - k^2)^{-1}$ result is left to the reader (Problem 65). ∎

Now suppose that $|V(x)| \leq ce^{-2a|x|}$. Then clearly $V: X_{-a} \to X_a$ is bounded so that $V(-\Delta - k^2)^{-1}$ is, for each k, a compact operator from X_a to itself. Moreover, $\eta = -V(-\Delta - k^2)^{-1}\eta$ has no solutions in X_a for $\operatorname{Im} k > 0$, $\arg k \neq \frac{1}{2}\pi$ since it has no solutions in L^2 for, if $\varphi \in L^2$ obeys the equation, then $\psi = (-\Delta - k^2)^{-1}\varphi$ is in $D(H)$ and obeys $(-\Delta + V)\psi = k^2\psi$. It follows by the analytic Fredholm theorem that except for a discrete set $\mathscr{E} \subset \mathbb{R}$, $(1 + V(-\Delta - k^2)^{-1})^{-1}$ has an analytic continuation from $\operatorname{Im} k > 0$ to a neighborhood N of $\mathbb{R}$ with $\mathscr{E}$ removed. Since $(H - k^2)^{-1} = (-\Delta - k^2)^{-1}(1 + V(-\Delta - k^2)^{-1})^{-1}$, we have proven case (a) of the following theorem. We shall use case (b) in Section 11.

Theorem XI.45 Let H be one of the following operators on $L^2(\mathbb{R}^n)$:

(a) $H = -\Delta + V$ with $|V(x)| \leq Ce^{-2a|x|}$.

(b) $H\eta = -\alpha\nabla \cdot \beta\nabla(\alpha\eta)$ with α and β strictly positive functions so that $\alpha - \alpha_0, \beta - \beta_0 \in C_0^\infty$ for suitable constants $\alpha_0, \beta_0 > 0$.

Then H is self-adjoint on $D(-\Delta)$ and there is a discrete set $\mathscr{E} \subset \mathbb{R}$ and a neighborhood N of $\mathbb{R}$ so that $(H-k^2)^{-1}$ has a continuation as an analytic $\mathscr{L}(X_a, X_{-a})$-valued function from the region $\{k \mid \operatorname{Im} k > 0,\ -k^2$ not an eigenvalue of $H\}$ to $N \backslash \mathscr{E}$. a is arbitrary in case (b).

Proof We need only prove case (b). By using Leibnitz' rule, we can write

$$H = -f\Delta + \mathbf{g} \cdot \nabla + h$$

where $\mathbf{g}$, h, $f_1 \equiv f - f_0 \in C_0^\infty$ and $f_0 = \alpha_0^2 \beta_0$. Moreover, $f = \alpha^2 \beta$ is strictly positive. That H is self-adjoint on $D(-\Delta)$ is a simple application of Theorem X.13 which we leave to the reader (Problem 66). Let $V = H - H_0$; $H_0 = -f_0 \Delta$. As above, the theorem will be proven if we show that $(1 + V(H_0 - k^2)^{-1})^{-1}$ is an analytic $\mathscr{L}(X_a, X_a)$-valued function. $V(H_0 - k^2)^{-1}$ is not compact but, if $W = g \cdot \nabla + h$, then

$$\begin{aligned} 1 + V(H_0 - k^2)^{-1} &= (H_0 + V - k^2)(H_0 - k^2)^{-1} \\ &= [ff_0^{-1}(H_0 - k^2) + W + k^2 f_1 f_0^{-1}](H_0 - k^2)^{-1} \\ &= ff_0^{-1} + [(W + k^2 f_1 f_0^{-1})(H_0 - k^2)^{-1}] \\ &= (ff_0^{-1})[1 + (f^{-1} f_0 W + f^{-1} f_1 k^2)(H - k^2)^{-1}] \end{aligned}$$

The expression in $[\cdots]$ is I plus an analytic function with values in the compact operators in $\mathscr{L}(X_a)$, so $I + V(H_0 - k^2)^{-1}$ is invertible except on a discrete set by Theorem VI.14. ∎

We now turn to producing eigenfunction expansions for $-d^2/dx^2 + V(x)$ with $|V(x)| \leq Ce^{-2a|x|}$. The key to all such expansions is the following heuristic formula:

$$\operatorname{Im}(H - k^2 - i0)^{-1} = W(k)^* [\operatorname{Im}(H_0 - k^2 - i0)^{-1}] W(k) \tag{99}$$

where

$$W(k) = (1 + V(H_0 - k^2 - i0)^{-1})^{-1}$$

and

$$\operatorname{Im}(A - k^2 - i0)^{-1} = \lim_{\varepsilon \downarrow 0} (2i)^{-1} [(A - k^2 - i\varepsilon)^{-1} - (A - k^2 + i\varepsilon)^{-1}]$$

(99) is formally true because if $\operatorname{Im} z > 0$, if A is self-adjoint, and if $B = A + C$ is self-adjoint on $D(A)$, then

$$\begin{aligned} (B - z)^{-1} - (B - \bar{z})^{-1} &= 2(\operatorname{Im} z)(B - \bar{z})^{-1}(B - z)^{-1} \\ &= 2(\operatorname{Im} z)[(1 + C(A - z)^{-1})^{-1}]^* (A - \bar{z})^{-1} \\ &\quad \times (A - z)^{-1}(1 + C(A - z)^{-1})^{-1} \\ &= [(1 + C(A - z)^{-1})^{-1}]^* \\ &\quad \times [(A - z)^{-1} - (A - \bar{z})^{-1}](1 + C(A - z)^{-1})^{-1} \end{aligned} \tag{100}$$

so that (99) results if one can take $\operatorname{Im} z$ to zero. In the case at hand, (99) is valid for $k^2 \notin \mathscr{E}$ if we interpret $(H - k^2 - i0)^{-1}$ and $(H_0 - k^2 - i0)^{-1}$ as maps from X_a to X_{-a}, $W(k)$ as a map from X_a to X_a, and $W(k)^*$ as a map from X_{-a} to X_{-a}. For these interpretations can be made if $k^2 - i0$ is replaced by z with $\operatorname{Im} z > 0$, and all maps are analytic up to $k^2 + i0$ (except in $\mathscr{E}$) so that (100) implies (99).

To supplement (99) we need the fact that $H_0 = -d^2/dx^2$ has an eigenfunction expansion with eigenfunctions $\varphi_0(x, k) = e^{ikx}$. Notice that these eigenfunctions lie in X_{-a} and that since the kernel of $(H_0 - k^2 - i0)^{-1}$ is $\frac{1}{2}e^{ik|x-y|}$, we have that for $f \in X_a$,

$$\begin{aligned} &\operatorname{Im}(f, (H_0 - k^2 - i0)^{-1} f) \\ &\quad = \frac{1}{2} \iint \overline{f(x)} \sin(k(x - y)) f(y)\, dx\, dy \\ &\quad = \tfrac{1}{2}[(f, \varphi_0(k))(\varphi_0(k), f) + (f, \varphi_0(-k))(\varphi_0(-k), f))] \end{aligned}$$

Defining $\varphi(k) = W(|k|)\varphi_0(k)$, we see by (99) that

$$\operatorname{Im}(f, (H - k^2 - i0)^{-1} f) = \frac{1}{2} \sum_{\delta = \pm 1} |(\varphi(\delta k), f)|^2$$

Using Stone's formula, we obtain that for $f \in X_a$ and $[a, b] \subset [0, \infty) \backslash \mathscr{E}$,

$$(f, P_{[a,b]} f) = \int_{a < k^2 < b} |f^*(k)|^2\, dk$$

where $f^*(k) = (2\pi)^{-1/2}(\varphi(k), f)$. From this point onward, the easy passage to the Plancherel relation and inversion formula for # and the connection with scattering theory are essentially identical to our discussion in Section 6.

XI.7 Quantum scattering IV: Dispersion relations

Rigorous proofs of dispersion relations are like breasts on a man, neither useful nor ornamental.
M. L. Goldberger

In agreement with the scheme presented at the conclusion of Section 5, we have seen that the two-body scattering operator has a "kernel," $\delta(\mathbf{k}-\mathbf{k}') - 2\pi i\delta(k^2-(k')^2)T(\mathbf{k},\mathbf{k}')$ where $T(\mathbf{k},\mathbf{k}')$ is continuous on $F \equiv \{\langle \mathbf{k},\mathbf{k}'\rangle \,|\, k^2 = (k')^2;\ k^2 \notin \mathscr{E}\}$. In this section we shall study T further. Our main goal will be to show that T is analytic in a suitable neighborhood of F when V lies in a somewhat restrictive class of potentials. To illustrate our method and to show that the analyticity of $T(\mathbf{k},\mathbf{k})$ is a general phenomenon, we first prove:

Theorem XI.46 Let V be in $L^1 \cap R$ and let $\mathbf{e}$ be a fixed unit vector in $\mathbb{R}^3$. Then, there exists a function $\tau_F(k)$ meromorphic in $\{k \,|\, \operatorname{Im} k > 0\}$ so that:

(a) If k_0 is real and $k_0^2 \notin \mathscr{E}$, then

$$\lim_{k\to k_0;\ \operatorname{Im} k>0} \tau_F(k) = T(k_0\mathbf{e}, k_0\mathbf{e})$$

The limit is uniform on compact subsets of $\mathbb{R}\backslash\mathscr{E}^{1/2}$.

(b) The only poles of τ_F in the upper half-plane occur on the imaginary axis at the points k where k^2 is an eigenvalue of $-\Delta + V$. Moreover all these poles are simple.

(c) $\tau_F(-\bar{k}) = \overline{\tau_F(k)}$.

(d) $\lim_{k\to\infty} \tau_F(k) = \tau_{\text{Born}} \equiv (2\pi)^{-3}\int V(x)\,dx$. The limit holds uniformly in the closed half-plane when τ_F is extended to $\mathbb{R}\backslash\mathscr{E}^{1/2}$

Proof For k real, define $\tau_F(k) = T(ke, ke)$. We want to find some kind of continuation of $\tau_F(k)$ to the upper half-plane. We know that for k real

$$\tau_F(k) = (2\pi)^{-3}\int e^{-ike\cdot x}V^{1/2}(x)\psi(x, ke)\,dx \tag{101}$$

where ψ solves the modified Lippmann–Schwinger equation (84). The kernel of (84) can be continued to the upper half k plane, but the homogeneous term $|V(x)|^{1/2}e^{ike\cdot x}$ may not be in L^2 if $\operatorname{Im} k \neq 0$. Therefore, we further modify the Lippmann–Schwinger equation. Noticing that $e^{-ike\cdot x}\psi(x, ke)$ is the quantity that enters in (101), we define

$$\chi(x, k) = e^{-ike\cdot x}\psi(x, ke)$$

Then

$$\tau_F(k) = (2\pi)^{-3}\int V^{1/2}(x)\chi(x, k)\,dx \tag{102a}$$

and χ solves

$$\chi(x, k) = |V(x)|^{1/2} + \int M(x, y; k)\chi(y, k)\,dy \tag{102b}$$

with

$$M(x, y; k) = -(4\pi|x-y|)^{-1}|V(x)|^{1/2}V^{1/2}(y)\exp\{ik[|x-y| - e\cdot(x-y)]\} \tag{102c}$$

Since $|(x-y)\cdot e| \le |x-y|$ for all x and y, $M(x, y; k)$ defines a Hilbert–Schmidt operator M_k for any k with $\operatorname{Im} k \ge 0$. A side argument (Problem 68) proves that $M_k\psi = \psi$ has a solution if and only if $K_k\varphi = \varphi$ has a solution where K_k is $-|V|^{1/2}(H_0 - k^2)^{-1}V^{1/2}$. It can also be shown that if $K_k\varphi = \varphi$ with $\operatorname{Im} k > 0$, then $\eta = (H_0 - k^2)^{-1}V^{1/2}\varphi \in Q(-\Delta + V)$ and $(H_0 + V)\eta = k^2\eta$ (Problem 69). Thus, by the analytic Fredholm theorem (Theorem VI.14), $(I - M_k)^{-1}$ exists except at the points k^2 that are eigenvalues of $-\Delta + V$ and $(I - M_k)^{-1}$ is meromorphic in the upper half-plane. Using the simplicity of the poles of $(-\Delta + V - k^2)^{-1}$, it can be shown that $(I - M_k)^{-1}$ has simple poles (Problem 71). For k in the upper half-plane, define

$$\tau_F(k) = (2\pi)^{-3}(V^{1/2}, (1 - M_k)^{-1}|V|^{1/2})$$

(a) and (b) are now easy.

As $k \to \infty$ in the closed half-plane, $\|M_k\| \to 0$ (see Problem 60), so (d) holds. Finally, if k is purely imaginary, each term in the series obtained by iterating (102b) is real-valued and the series converges if $|k|$ is large. Thus $\overline{\tau_F(-\bar{k})} = \tau_F(k)$ if $|k|$ is large and $\operatorname{Re} k = 0$. (c) follows by analytic continuation. ∎

In the case where V is spherically symmetric, τ_F is independent of $\mathbf{e}$ and $f(\mathbf{k}) = -2\pi^2\tau_F(\mathbf{k})$ is called the **forward scattering amplitude**. We saw in the last section that $\operatorname{Im}\tau_F(\mathbf{k})$ is determined by the total scattering cross section and unitarity. Interestingly enough, $\operatorname{Re}\tau_F(k)$ is determined by $\operatorname{Im}\tau_F(k)$ and a finite number of parameters, one for each bound state energy. For simplicity, consider the case where $\mathscr{E} = \varnothing$. Then:

Corollary If $V \in R \cap L^1(\mathbb{R}^3)$, if $\mathscr{E} = \varnothing$, and if we write $f(E) = -(2\pi)^2 \tau_F(\sqrt{E})$ for E real and positive, then

$$\operatorname{Re} f(E) = \mathscr{P} \int_0^\infty \frac{\operatorname{Im} f(E')}{E' - E} \frac{dE'}{\pi} + f_{\text{Born}} + \sum_{j=1}^{n} \frac{r_j}{E_j - E} \tag{103}$$

where $\mathscr{P} \int_0^\infty$ is the Cauchy principle value integral, $f_{\text{Born}} = -(4\pi)^{-1} \int V(x)\, dx$ and $E_1, \ldots, E_n$ are the bound states of $-\Delta + V$.

Sketch of proof This is a simple application of the analyticity of Theorem XI.46; the details are left to the reader (Problem 72). $f(E)$ is analytic in the plane with the positive reals and with the points $E_1, \ldots, E_n$ removed. Let E have positive real and imaginary parts. By the Cauchy integral theorem,

$$f(E) - f_{\text{Born}} = \frac{1}{2\pi i} \oint_C \frac{f(E') - f_{\text{Born}}}{E' - E}\, dE'$$

where C is the contour in Fig. XI.9. Since $f(E') - f_{\text{Born}} \to 0$ as $E' \to \infty$, the

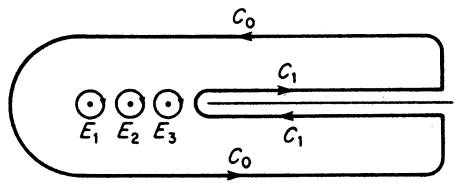


FIGURE XI.9 A contour of integration.

part of the contour marked C_0 makes no contribution as we move it out toward infinity. Thus

$$f(E) = f_{\text{Born}} + \frac{1}{2\pi i} \oint_{C_1} \frac{f(E') - f_{\text{Born}}}{E' - E}\, dE' + \sum_{j=1}^{n} \frac{2r_j}{E_j - E}$$

Fix E_0 on the real axis, let $E = E_0 + i\varepsilon$ and let $\varepsilon \downarrow 0$. Using $\lim_{\varepsilon \downarrow 0} (x - E_0 - i\varepsilon)^{-1} = \mathscr{P}(x - E_0)^{-1} + i\pi\delta(x - E_0)$, see (V.4), (103) results. ∎

(103) is called a **forward dispersion relation.** One of the intriguing aspects of forward dispersion relations and of the analyticity of τ_F is the connection exhibited between scattering and bound states. In particular, if we measure $f(E)$, the forward scattering amplitude, we can determine the bound state energies (or at least those with $r_j \neq 0$) by using (103). This connection between scattering and bound states will be further exhibited in Levinson's theorem (Theorem XI.59).

Our discussion of more general analyticity will require that the potential V fall off exponentially in the sense that $Ve^{\alpha|x|} \in L^1 \cap R$ for some $\alpha > 0$. For simplicity, we shall also suppose that V is spherically symmetric. In that case, the function $T(\mathbf{k}, \mathbf{k}')$ depends only on the two variables $E = k^2$ and $\cos\theta = \mathbf{k} \cdot \mathbf{k}'/E$ in the region $F \cap \{\langle \mathbf{k}, \mathbf{k}' | k = k' \rangle$. Alternatively, one often uses the variable Δ given by $\Delta^2 \equiv \frac{1}{2}(\mathbf{k} - \mathbf{k}')^2 = \frac{1}{2}E(1 - \cos\theta)$. The "physical" regions in the variables $\langle E, \cos\theta \rangle$ or $\langle E, \Delta \rangle$ are the images of $\{\langle \mathbf{k}, \mathbf{k}' \rangle \in \mathbb{R}^6 | k = k'\}$; explicitly, $\{\langle E, \cos\theta \rangle | 0 \leq E < \infty;\ -1 \leq \cos\theta \leq 1\}$ and $\{\langle E, \Delta \rangle | 0 \leq E < \infty,\ 0 \leq \Delta \leq \sqrt{E}\}$. It is also useful to consider the Born term

$$f_B(\Delta) = -(4\pi)^{-1} \int e^{-2i\Delta \mathbf{e} \cdot \mathbf{x}} V(x)\, d\mathbf{x}$$

For any fixed unit vector $\mathbf{e}$, $f_B(\Delta)$ is independent of $\mathbf{e}$. If $Ve^{\alpha|x|} \in L^1$, then $f_B(\Delta)$ is analytic in the region $|\operatorname{Im} \Delta| < \frac{1}{2}\alpha$. The general analyticity result is:

Theorem XI.47 Suppose that $Ve^{\alpha|x|} \in R$ for some $\alpha > 0$. Let $f(k, \Delta)$ be the scattering amplitude defined in the region $G \equiv \{\langle k, \Delta \rangle | k \geq 0,\ k^2 \notin \mathscr{E},\ 0 \leq \Delta \leq k^2\}$. Let $0 < \beta \leq \alpha$ and let

$$D_\beta = \Big\{ \langle k, \Delta \rangle \in \mathbb{C}^2 \Big| |\operatorname{Im} \Delta| < \beta,\ 4 \operatorname{Im} k > \alpha - \beta,$$
$$|\operatorname{Im} \sqrt{k^2 - \Delta^2}| - |\operatorname{Im} k| < \sqrt{\alpha^2 - (\operatorname{Im} \Delta)^2} \Big\}$$

and let $D = \bigcup_{0 < \beta \leq \alpha} D_\beta$. Then there exists a function $g(k, \Delta)$, meromorphic in D, such that if $\langle k, \Delta \rangle \in G$, then $G(k, \Delta) = f(k, \Delta) - f_{\text{born}}(\Delta)$. Moreover, g has no poles in $D \cap \{\langle k, \Delta \rangle | k \in \mathbb{R}\}$ and the only poles in $D \cap \{\langle k, \Delta \rangle | \operatorname{Im} k > 0\}$ occur at points k where k^2 is an eigenvalue of $H_0 + V$. In particular:

(a) $f(k, \Delta)$ has an analytic continuation to a neighborhood of the physical region, and the exceptional points $\mathscr{E}$ are removable singularities.

(b) Let $h(k, z)$ be g in the new variable $z = 1 - 2k^{-2}\Delta^2$, so that $z = \cos\theta$ in the physical region. Then, for fixed k, $h(k, z)$ is analytic in the ellipse centered at $z = 0$ with foci at $z = \pm 1$, and with semimajor axis $1 + 2k^{-2}\alpha^2$. This is called the **Lehmann ellipse.**

For a proof, the reader can consult the reference given in the Notes. The main idea, already used in the proof of Theorem XI.46, is the definition of a suitably modified Lippmann–Schwinger equation. To prove that the exceptional set $\mathscr{E}$ is removable, one uses unitarity and the partial wave expansion

discussed in the next section. Because the Lehmann ellipse will be used in the next section, let us show that it lies in D. Fix k real. Then $\langle k, \Delta\rangle \in D$ if and only if $(\operatorname{Im}\Delta)^2 + (\operatorname{Im}\sqrt{k^2 - \Delta^2})^2 < \alpha^2$. But $\Delta = k\sqrt{\frac{1}{2}(1-z)}$ and $\sqrt{k^2 - \Delta^2} = k\sqrt{\frac{1}{2}(1+z)}$. Thus $\langle k, \Delta\rangle \in D$ if and only if

$$(\operatorname{Im}\sqrt{1-z})^2 + (\operatorname{Im}\sqrt{1+z})^2 < 2\alpha^2/k^2$$

Since $|w|^2 = \operatorname{Re}(w^2) + 2(\operatorname{Im} w)^2$, we see that this is equivalent to

$$|1-z| + |1+z| < 4\alpha^2 k^{-2} + \operatorname{Re}(1-z) + \operatorname{Re}(1+z)$$
$$= 2(1 + 2\alpha^2 k^{-2})$$

This is precisely the ellipse in question.

Finally, we describe the strong analyticity results which hold for potentials of a special form:

Definition A **generalized Yukawa potential** is a spherically symmetric function on $\mathbb{R}^3$ of the form

$$V(r) = \sum_{j=0}^{N} r^{j-1} \int_{\mu_0}^{\infty} e^{-\mu r}\, d\rho_j(\mu)$$

where $\mu_0 > 0$, N is a finite integer, and $\rho_0, \ldots, \rho_N$ are real (but not necessarily positive) measures of finite total variation.

These potentials are "superpositions" of the basic **Yukawa potential** $r^{-1}e^{-\mu r}$ for notice that $V(r) = y^{-1}\int_{\mu_0}^{\infty} e^{-\mu r} T(\mu)\, d\mu$ where T is the distribution $T = \sum_{j=0}^{N} D^j \rho_j$. Generalized Yukawa potentials have several basic properties: (i) Since $r|V(r)| \leq e^{-\mu r}\sum_{j=0}^{N} \|\rho_j\| r^j$ is bounded by $Ce^{-\frac{1}{2}\mu_0 r}$, V is in $L^2(\mathbb{R}^3)$. Thus $-\Delta + V$ is self-adjoint on $D(-\Delta)$. (ii) V falls off exponentially, so Theorem XI.47 is applicable. (iii) $V(r)$ has an analytic continuation to the region $\{r \mid |\arg r| < \frac{1}{2}\pi\}$ and for any real θ with $|\theta| < \frac{1}{2}\pi$, $V_\theta(r) \equiv V(e^{i\theta}r)$ is in L^2. This last property will play an important role in Sections XI.8 and XIII.10. It is also important in the proof of the following analyticity result:

Theorem XI.48 Let $f(k, \Delta)$ be the scattering amplitude associated with a generalized Yukawa potential. Fix k real. Then $f(k, \Delta)$ has an analytic continuation to the region of the $z(= \cos\theta)$-plane $\{z \mid z \notin [\zeta(k), \infty)\}$ where $\zeta(k) = 1 + 2k^{-2}\mu_0^2$.

This analyticity is one of several properties of f that we discuss in the Notes.

XI.8 Quantum scattering V: Central potentials

In this section we discuss some aspects of the two-body case when the potential is spherically symmetric, that is, a function only of $|x|$. Such potentials are called **central potentials**. The material that we present primarily involves the additional structure present in the central case. However, we remark that many results of the scattering theory we have already developed and of the spectral theory of Chapter XIII can be more easily proved and generalized in the central case; see for example Theorem XI.31 and Appendix 3 to this section. In the Notes to this section, we present a guide to the literature on these aspects of central potentials.

Because the subjects that we discuss are quite distinct, the section is divided into six parts: (A) We discuss the reduction of the S-operator due to symmetries. (B) This will lead us to a formal partial wave expansion of the scattering amplitude $f(E, \theta)$. Using analyticity in the Lehmann ellipse, we shall prove that the partial wave expansion converges *uniformly* when $Ve^{\alpha|x|} \in R$ for some $\alpha > 0$. (C) We shall relate the partial wave amplitudes to a quantity, called the phase shift, defined by the time-independent radial Schrödinger equation. (D) We study a nonlinear first order differential equation which yields the s-wave phase shift. (E) We develop the Jost function method of discussing the s-wave partial wave amplitude, and, in particular, we shall prove Levinson's theorem which relates the number of bound states to scattering data. (F) When V is a generalized Yukawa potential, we study the analyticity properties of the s-wave amplitude.

Except for a brief discussion in the Notes, we shall not treat continuation in angular momentum and Regge theory. In many ways, the central theorem of the section is Theorem XI.54. Some important properties of certain special functions are collected in Appendix 1. Jost functions for certain oscillatory potentials are studied in Appendix 2.

A. Reduction of the S-matrix by symmetries

We begin with the N-body case and then specialize to the two-body case. We already know that the S-operator commutes with the free energy H_0 (by a proposition preceding Theorem XI.33). If V is a central potential, then both H and H_0 commute with rotations. Thus the wave operators $\Omega^{\pm}$ and therefore the S-operator commute with rotations. In order to summarize, we make a technical definition, expressing the "natural" action of rotations on the asymptotic Hilbert space, $\mathscr{H}_{\text{asym}}$ of Section 5.

Definition Let $\mathscr{C}$ be a listing of all channels of an N-body quantum system with the proviso on degenerate eigenvalues. Fix a cluster decomposition D and an energy E and let $\mathscr{C}_1 \subset \mathscr{C}$ be the family of channels, with $D(\alpha) = D$ and $E(\alpha) = E$. Thus a channel $\alpha \in \mathscr{C}_1$ has the form

$$\alpha = \begin{pmatrix} C_1 & \cdots & C_k \\ \eta_1^{(i_1)} & \cdots & \eta_k^{(i_k)} \end{pmatrix}$$

where $\{\eta_\ell^{(i_\ell)}\}_{i_\ell}$ for ℓ fixed is an orthonormal family. Given α, $\beta \in \mathscr{C}_1$ let $J_{\beta\alpha}: \mathscr{H}_\alpha \to \mathscr{H}_\beta$ be the natural identification. Given $R \in SO(3)$, the group of three-dimensional rotations, and a function η, let $\eta \circ R^{-1}$ denote the function $(\eta \circ R^{-1})(x) = \eta(R^{-1}x)$. Since the clustered channel Hamiltonians commute with rotations, each $\eta_\ell^{(i_\ell)}$ composed with R is a linear combination

$$\eta_\ell^{(i_\ell)} \circ R^{-1} = \sum_j D_\ell^{(i_\ell, j_\ell)}(R)\eta_\ell^{(j_\ell)}$$

of the other $\eta_\ell^{(j_\ell)}$. Let $V_\alpha(R)$ denote the natural action of the rotations on $\mathscr{H}_\alpha \equiv L^2(\mathbb{R}^{3k-3})$. Then define $U_R^{(\alpha)}: \mathscr{H}_\alpha \to \oplus_{\beta \in \mathscr{C}_1} \mathscr{H}_\beta$ by

$$U_R^{(\alpha)} = \sum_{j_1, \ldots, j_k} \left(\prod_{\ell=1}^{k} D^{(i_\ell, j_\ell)}(R) \right) J_{\beta\alpha} V_\alpha(R)$$

where β is the channel

$$\beta = \begin{pmatrix} C_1 & \cdots & C_k \\ \eta_1^{(j_1)} & \cdots & \eta_k^{(j_k)} \end{pmatrix}$$

Finally, U_R is defined from $\oplus_{\alpha \in \mathscr{C}} \mathscr{H}_\alpha \to \oplus_{\alpha \in \mathscr{C}} \mathscr{H}_\alpha$ by $U_R \restriction \mathscr{H}_\alpha \equiv U_R^{(\alpha)}$.

Proposition 1 Let S be the S-operator of an N-body quantum system satisfying the hypotheses of Theorem XI.34 with center of mass removed. Then S commutes with $\exp(itH_{\text{asym}})$ for all $t \in \mathbb{R}$. If all the V_{ij} are central, then S commutes with all rotations, that is, $SU_R = U_R S$ for all $R \in SO(3)$.

In the classical case, we saw that symmetries considerably simplified the S-operator; a priori, the classical S-matrix was a map from $\mathbb{R}^6$ to $\mathbb{R}^6$. By using symmetries, we were able to describe S as a function from $\mathbb{R}_+ \times \mathbb{R}_+$ to $\mathbb{R} \times [0, \pi]$. We shall find the restrictions that symmetries place on the quantum-mechanical S-operator. First we study the effect of energy conservation by giving a general proposition about operators commuting with a one-parameter group.

Definition Let $\langle M, \mu \rangle$ be a σ-finite measure space, let $\mathscr{H}_0$ be a separable Hilbert space, and let $\mathscr{H} = L^2(M, d\mu; \mathscr{H}_0)$. We say that a function a from M to $\mathscr{L}(\mathscr{H}_0)$, the bounded operators on $\mathscr{H}_0$, is *measurable* if $(\psi, a(\cdot)\varphi)$ is measurable for each ψ, $\varphi \in \mathscr{H}_0$. We say that $a \in L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}_0))$ if a is measurable and ess.sup. $\|a(\cdot)\|_{\mathscr{L}(\mathscr{H}_0)} < \infty$. Given $a \in L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}_0))$, there is, by the Riesz lemma, an operator $A \in \mathscr{L}(\mathscr{H})$ so that for each ψ, $\varphi \in \mathscr{H}$,

$$(\psi, A\varphi)_{\mathscr{H}} = \int_M (\psi(\lambda), a(\lambda)\varphi(\lambda))_{\mathscr{H}_0} \, d\mu(\lambda)$$

We call such a map a **decomposable operator** and call $a(\lambda)$ **the fiber of A at λ.** A determines its fibers a.e.

Fibered operators are further discussed in Section XIII.16 where the Riesz lemma argument occurs as part of Theorem XIII.83.

Proposition 2 Let $\mathscr{H}_0$ be a separable Hilbert space and let μ be a Borel measure on $\mathbb{R}$. Let B be multiplication by x on $L^2(\mathbb{R}, d\mu; \mathscr{H}_0) \equiv \mathscr{H}$. Suppose that $A \in \mathscr{L}(\mathscr{H})$ commutes with e^{itB} for each $t \in \mathbb{R}$. Then A is a decomposable operator. Moreover, if A is unitary (respectively, self-adjoint), then its fibers are (a.e.) unitary (respectively, self-adjoint) operators on $\mathscr{H}_0$.

The first part of the proposition is a special case of Theorem XIII.84. The second part is easy since A and its fibers are bounded.

Example 1 Let S be the S-matrix for scattering from a reduced two-body system of reduced mass $\frac{1}{2}$ on $L^2(\mathbb{R}^m) = \mathscr{H}$. Suppose that S is unitary. Let $\mathscr{H}_0$ be the Hilbert space $L^2(S^{m-1}; d\Omega)$ where S^{m-1} is the unit sphere in $\mathbb{R}^m$ and $d\Omega$ is its standard surface measure. Define the unitary map $U: L^2(\mathbb{R}^m) \to L^2(\mathbb{R}_+, dE; \mathscr{H}_0)$ by

$$[(Uf)(E)](\omega) = (\sqrt{2})^{-1} E^{(m-2)/4} \hat{f}(E^{1/2}\omega) \tag{104}$$

where $\omega \in S^{m-1}$ is viewed as a unit vector in $\mathbb{R}^m$. When we are given an operator A on $L^2(\mathbb{R}^m)$, we shall call UAU^{-1} "the operator A in the energy representation." In the energy representation, H_0 is multiplication by E, so that Proposition 2 above is applicable to S by Proposition 1. Thus, in the energy representation, S is a decomposable operator whose fibers $S(E)$ are unitary maps of $L^2(S^{m-1}, d\Omega)$ to itself. We define $T(E)$ by

$$T(E) = (2\pi i)^{-1}(I - S(E))$$

In case $m = 3$ and $V \in L^1 \cap R$, Theorem XI.42 provides an explicit representation for $T(E)$, namely

$$(T(E)f)(\omega) = \frac{E^{1/2}}{2} \int_{S^{m-1}} T(E^{1/2}\omega, E^{1/2}\omega')f(\omega')\, d\Omega(\omega') \tag{105}$$

where $T(\cdot, \cdot)$ is the "T-matrix." We shall pursue this realization of $T(E)$ as an integral operator below.

Example 2 Let $\mathscr{H}_{\text{asym}}$ be the asymptotic Hilbert space for an N-body quantum system on $L^2(\mathbb{R}^{3N-3})$. Recall that for each $\alpha \in \mathscr{C}$, an index set for the channels, we defined the channel energy E_α to be the sum of the internal energy of the clusters in α. E_α is sometimes called the **threshold for channel α**. For each $E \in \mathbb{R}$, the set

$$\mathscr{C}_E = \{\alpha \in \mathscr{C} \mid E_\alpha < E\}$$

is called the **set of open channels** at energy E. Let α be an ℓ-cluster channel so that the channel Hilbert space $\mathscr{H}_\alpha = L^2(\mathbb{R}^{3\ell-3})$. As in the two-body case (Example 1), we can realize H_α as multiplication by $(E + E_\alpha)$ on $L^2(\mathbb{R}_+, dE; L^2(S^{3\ell-4}, d\mu_\alpha))$ although μ_α and the explicit formula for the energy representation are more complicated than (104) because of the possible different masses of different clusters. Next suppose that one can write $[E, \infty) = \bigcup_{n=1}^{\infty} I_n$ where: (1) $E = \inf \sigma(H)$; (2) the I_n are disjoint intervals; (3) for each fixed n, the set $\mathscr{C}_E$ is the same for each $E \in I_n$. Such a decomposition exists so long as H has "reasonable" spectral properties, for example, if each subsystem has $\sigma_{\text{pp}}(H(C)) = \sigma_{\text{disc}}(H(C))$ or if each $H(C)$ has eigenvalues that cluster only at thresholds (Problem 74); in Section XIII.10 we shall see that such spectral properties can sometimes be proven. Let $\{P_\Omega\}$ be the spectral projections for H_{asym} and write $\mathscr{H}_{\text{asym}} = \oplus_{n=1}^{\infty} \mathscr{H}^{(n)}$ where $\mathscr{H}^{(n)} = \text{Ran } P_{I_n}$. Since S commutes with each P_Ω, it leaves each $\mathscr{H}^{(n)}$ invariant. It is now possible to apply Proposition 2 and obtain a fibering of each $S \upharpoonright \mathscr{H}^{(n)}$. One can think of S itself as a generalized decomposable operator, but the fibers $S(E)$ are maps on Hilbert spaces with some E dependence; explicitly $S(E)$ is a map on $\mathscr{H}_E \equiv \oplus_{\alpha \in \mathscr{C}_E} \mathscr{H}_\alpha^{(0)}$ where $\mathscr{H}_\alpha^{(0)} = L^2(S^{3\ell-4}, d\mu_\alpha)$. As E is increased, the Hilbert space $\mathscr{H}_E$ on which the fibers act increases each time a new scattering threshold is passed. We remark that the energy representation we have just described where the space $\mathscr{H}_E$ is not independent of E is discussed most naturally in the language of direct integrals of Hilbert spaces.

Before turning to the consequences of rotational invariance, we want to study the operators $T(E)$ of Example 1 in more detail:

Theorem XI.49 Let $H = -\Delta + V$ where V is in R. Then:

(a) For each $E \in \mathbb{R}_+ \backslash \mathscr{E}$, the map $T(E)$ on $L^2(S^2, d\Omega)$ is Hilbert–Schmidt.
(b) $E \to T(E)$ is a continuous map from $\mathbb{R}_+ \backslash \mathscr{E}$ to the Hilbert–Schmidt operators with their natural topology.
(c) As $E \to \infty$, $T(E) \to 0$ in operator norm.

If, moreover, V is in L^1, then "Hilbert–Schmidt" in (a) and (b) can be replaced with "trace class."

Proof For each $E > 0$, let $K_V(E)$ be the Hilbert–Schmidt operator on $L^2(\mathbb{R}^3)$ with kernel

$$\frac{|V(x)|^{1/2} e^{i\sqrt{E}|x-y|} V(y)^{1/2}}{4\pi|x-y|}$$

and let $F_V(E)$ be the map from $L^2(\mathbb{R}^3)$ to $L^2(S^2, d\Omega)$ given by

$$(F_V(E)f)(\omega) = \tfrac{1}{4} E^{1/4} \pi^{-3/2} \int \exp(-iE^{1/2}\omega \cdot x) V^{1/2}(x) f(x)\, dx \tag{106}$$

Our main tool will be to show that $F_V(E)$ is a bounded operator in the class $\mathscr{I}_4$ (defined in the Appendix to Section IX.4) and that

$$T(E) = F_V(E)[I + K_V(E)]^{-1} F_{|V|}(E)^* \tag{107}$$

for all $E \in \mathbb{R}_+ \backslash \mathscr{E}$. (107) is intimately related to (99). We shall need the formula

$$(F_V(E)^* g)(x) = \tfrac{1}{4} E^{1/4} \pi^{-3/2} \int \exp(+iE^{1/2}\omega \cdot x) V^{1/2}(x) g(\omega)\, d\Omega(\omega) \tag{108}$$

Suppose first that $V \in L^1 \cap R$. Then $T(E)$ is given as the integral operator (105) with

$$T(k, k') = (2\pi)^{-3} \int V(x)^{1/2} e^{-ik \cdot x} \psi(x, k')\, dx$$

where

$$\psi(\cdot, k) = [I + K_V(k^2)]^{-1} \psi_0(\cdot, k)$$

and

$$\psi_0(x, k) = |V(x)|^{1/2} \exp(ik \cdot x)$$

As a result, (107) is proven in this case.

We next need the following properties of $F_V(E)$ whose proofs are left to the reader (Problem 75):

(1) When $V \in R$, $F_V(E) \in \mathscr{I}_4$, that is, $F_V(E)^* F_V(E)$ is Hilbert–Schmidt.
(2) $E \to F_V(E)$ is continuous in the $\mathscr{I}_4$ topology.
(3) For fixed $E \neq 0$, $V \to F_V(E)$ is continuous from the class of Rollnik potentials with their natural norm to $\mathscr{I}_4$.

(1′)–(3′) If R is replaced by $L^1 \cap R$ and $\mathscr{I}_4$ by $\mathscr{I}_2$, (1)–(3) still hold.

For example, the explicit formula (106) shows that $F_V(E)$ has an L^2 kernel when $V \in L^1$ (proving (1′)) and the explicit formula

$$(F_V(E)^* F_V(E) g)(x) = \int \frac{V(x)^{\ddagger} V(y)^{\ddagger}}{|x-y| 4\pi^2} \sin(E^{1/2}|x-y|) g(y)\, dy$$

proves (1).

In addition, we need a fact which is proven by combining the theory of smooth perturbations with the Kato–Birman theory (see Problem 57 of Chapter XIII):

(4) If $V_n \to V$ in Rollnik norm, then the corresponding S-matrices converge strongly.

Fix $V \in R$ and choose $V_n \in L^1 \cap R$ so that $V_n \to V$ in Rollnik norm. Suppose that $E_0 \in \mathbb{R}_+ \backslash \mathscr{E}$. Since we can find an interval A about E_0 so that $\bar{A} \cap \mathscr{E} = \varnothing$ and since the map $\langle V, E \rangle \mapsto K_V(E)$ of $R \times \mathbb{R}_+$ into $\mathscr{I}_2$ is jointly continuous (Problem 76), for all large n, A is disjoint from the exceptional set $\mathscr{E}_n$ for $-\Delta + V_n$. Since the S-matrices S_n converge to S (by (4)), since $F_{V_n}(E) \to F_V(E)$ (by (3)), and since we know that (107) holds for each V_n, it holds for V as long as $E \in A$. (a) and (b) now follow from (2) and (107). The proof of (c) is left to the reader (Problem 77). ∎

Using the method of weighted L^2 estimates (Section XIII.8), (107) and certain continuity properties of $T(E)$ can be extended to potentials behaving like $r^{-1-\varepsilon}$ at infinity (see the references in the Notes to Section XIII.8).

Since $T(E)$ is a Hilbert–Schmidt operator, it has an integral kernel $t(E; \omega, \omega')$. Because of a difference in normalization, t should be distinguished from the T-matrix T of Section 6; in fact, as we have seen (105):

$$t(E; \omega, \omega') = \tfrac{1}{2} E^{1/2} T(E^{1/2}\omega, E^{1/2}\omega')$$

when $V \in L^1 \cap R$. Unfortunately, this distinction between t and T is typical of obnoxious factors of $E^{1/2}$, 2π, -1, and i which continually crop up in scattering theory.

Suppose now that V is a central potential. Since S commutes with rotations, so does $T(E)$ for almost all E. Because $E \to T(E)$ is continuous on

$\mathbb{R}_+ \backslash \mathscr{E}$, we conclude that $T(E)$ commutes with rotations. Thus for every rotation R acting on S^2 and $E \in \mathbb{R}_+ \backslash \mathscr{E}$,

$$t(E; R\omega, R\omega') = t(E; \omega, \omega')$$

It follows that $t(E; \omega, \omega')$ is a function only of $\omega \cdot \omega' \equiv \cos\theta$. We state our final result in terms of the quantity f of (96) and (97), which is related to the differential cross section by $d\sigma/d\Omega = |f|^2$.

Definition $f(E, \cos\theta) = -(2\pi)^2 E^{-1/2} t(E; \omega, \omega')$ where $\omega \cdot \omega' = \cos\theta$. f is called the **scattering amplitude**.

We summarize the reduction due to symmetrics:

Theorem XI.50 Let $V \in R$ be a central potential and let S be the S-operator for $-\Delta + V$. Then there is a function $f(E, \cos\theta)$ from $(\mathbb{R}_+ \backslash \mathscr{E}) \times [-1, 1]$ to $\mathbb{C}$ so that the fibers of S, $S(E)$, have integral kernel:

$$(S(E) - I)(\omega, \omega') = \frac{i}{2\pi} E^{1/2} f(E, \omega \cdot \omega')$$

Thus the classical reduced S-function from $\mathbb{R}_+ \times \mathbb{R}_+$ to $\mathbb{R} \times [0, \pi]$ is replaced with a single *complex-valued* function on $\mathbb{R}_+ \times [0, \pi]$. If we separate f into its argument and magnitude, we obtain two real-valued functions. Since the scattering cross section depends only on the magnitude of f, this magnitude is the analogue of the classical scattering angle function in that it contains the same kind of physical information. In a sense which can be made precise, the argument of f contains time-delay information (see the references in the Notes).

B. The partial wave expansion and its convergence

We have just seen that $T(E)$ is a Hilbert–Schmidt operator. It is also normal because $S(E)$ is unitary. Thus $T(E)$ has a complete orthonormal set of eigenvectors. As a result, so does $S(E)$. If the potentials are central, we can identify the eigenvectors by using the rotational invariance! The group $SO(3)$ of rotations acting on $L^2(S^2, d\Omega)$ induces a decomposition of $L^2(S^2, d\Omega)$ into a direct sum $\oplus_{\ell=0}^{\infty} \mathscr{H}_\ell$ where $\mathscr{H}_\ell$ is the $(2\ell+1)$-dimensional subspace spanned by the spherical harmonics of order ℓ. Each subspace is left invariant by $SO(3)$ and the restriction of the action of $SO(3)$ to $\mathscr{H}_\ell$ is an

irreducible representation (see Section XVI.2 for the basic definitions and for Schur's lemma). The representations are inequivalent for distinct ℓ. It follows by Schur's lemma that $S(E)$ leaves each $\mathscr{H}_\ell$ invariant and that there exist numbers $s_\ell(E)$ so that for each $\psi \in \mathscr{H}_\ell$,

$$S(E)\psi = s_\ell(E)\psi$$

Definition The quantities $s_\ell(E)$ are called **partial wave S-matrix elements**. The quantities $f_\ell(E)$ defined by

$$f_\ell(E) = (2iE^{1/2})^{-1}[s_\ell(E) - 1] \tag{109}$$

are called **partial wave scattering amplitudes**.

Theorem XI.51 (partial wave expansion: L^2 convergence theorem) Let $V \in R$ be a central potential and fix $E \in \mathbb{R}_+ \backslash \mathscr{E}$. Then the partial wave amplitudes $f_\ell(E)$ and the scattering amplitude $f(E, \cos\theta)$ are related by

$$f(E, \cos\theta) = \sum_{\ell=0}^{\infty} (2\ell + 1) f_\ell(E) P_\ell(\cos\theta) \tag{110a}$$

$$f_\ell(E) = \tfrac{1}{2} \int_{-1}^{1} f(E, z) P_\ell(z)\, dz \tag{110b}$$

The sum in (110a) is convergent to $f(E, \cos\theta)$ in $L^2(S^2, d\Omega)$-norm for each fixed E. (110a) is called the **partial wave expansion**. The functions $P_\ell(z)$ are the Legendre polynomials. We summarize their properties in an appendix to this section.

Proof Let ω_0 be a fixed direction. Then $P_\ell(\omega \cdot \omega_0)$ is an element of the subspace $\mathscr{H}_\ell$, so

$$\int t(E; \omega, \omega') P_\ell(\omega' \cdot \omega_0)\, d\Omega(\omega') = (-2\pi i)^{-1}(s_\ell(E) - 1) P_\ell(\omega \cdot \omega_0)$$

Picking $\omega = \omega_0$ and using the formula defining $f(E; \omega \cdot \omega')$, we see that

$$\int f(E; \omega' \cdot \omega_0) P_\ell(\omega' \cdot \omega_0)\, d\Omega(\omega') = 4\pi f_\ell(E) P_\ell(1)$$

Since $P_\ell(1) = 1$ and $\int f(\omega')\, d\Omega(\omega') = 2\pi \int f(\omega')\, d(\omega' \cdot \omega_0)$ for functions f of $\omega' \cdot \omega_0$, (110b) results. On the other hand, since $t(E; \omega, \omega')$ is the kernel of a Hilbert–Schmidt operator, $\int_{-1}^{1} |f(E; z)|^2\, dz < \infty$. Since the $P_\ell(z)$ are a complete orthogonal family with $\int_{-1}^{1} |P_\ell(z)|^2\, dz = 2(2\ell + 1)^{-1}$, (110a) follows from (110b). ∎

The orthogonality relations for the P_ℓ functions have an important consequence. For, the total cross section is given by $\sigma = \int (d\sigma/d\Omega)\, d\Omega = 2\pi \int_{-1}^{1} |f(E; z)|^2\, dz$, so we obtain the basic formula

$$\sigma(E) = 4\pi \sum_{\ell=0}^{\infty} (2\ell + 1) |f_\ell(E)|^2 \tag{111}$$

It is sometimes possible to make a much stronger statement about the convergence of the partial wave expansion than we have in Theorem XI.51:

Theorem XI.52 (partial wave expansion; uniform convergence theorem) Let V be a central potential with $e^{\alpha|x|}V \in R$ for some $\alpha > 0$. Fix $E \in \mathbb{R}_+ \backslash \mathscr{E}$. Then the partial wave expansion (110a) converges uniformly for $\theta \in [0, 2\pi]$.

Proof By Theorem XI.47, $f(E, z)$ is analytic for z in the ellipse with foci ± 1 and semimajor axis $1 + 2\alpha^2 E^{-1}$. The uniform convergence of the partial wave expansion on compact subsets of this ellipse now follows from a general theorem on the convergence of Legendre series (Theorem XI.63 in Appendix 1). ∎

C. Phase shifts and their connection to the Schrödinger equation

In part B we did not make use of the fact that the S-matrix is unitary. This fact immediately implies that the numbers $s_\ell(E)$, which are eigenvalues of $S(E)$, have modulus one.

Definition The **phase shifts** $\delta_\ell(E)$, are defined by the equation

$$s_\ell(E) = e^{2i\delta_\ell(E)}$$

A priori, the phase shifts are real numbers defined for almost every E, and they are only determined modulo π. Let $E_0 = \max\{E \mid E \in \mathscr{E}\}$ where $\mathscr{E}$ is the exceptional set. Since $\lim_{E\to\infty} S(E) = I$ and $S(E)$ is continuous on (E_0, ∞), we can eliminate the a.e. and modulo π ambiguities for $E \in (E_0, \infty)$ by requiring that $\delta_\ell(E)$ be continuous there and that $\lim_{E\to\infty} \delta_\ell(E) = 0$. Under mild assumptions, we shall see in Sections D and E below that $s_0(E)$ and hence $\delta_0(E)$ can be chosen to be continuous on $[0, \infty)$. Similarly, one can also prove that $\delta_\ell(E)$ can be chosen continuous for $\ell > 0$. The phase shift, defined to be continuous in E and to obey $\lim_{E\to\infty} \delta_\ell(E) = 0$ for each fixed ℓ,

also obeys $\lim_{\ell\to\infty}\delta_\ell(E)=0$ for each fixed E. In fact, since $S(E)-I$ is Hilbert–Schmidt when $V\in R$, one has $\sum_{\ell=0}^{\infty}(2\ell+1)|\delta_\ell(E)|^2<\infty$ in that case.

The partial wave amplitude can now be written in three different ways, each of them useful in different contexts:

$$f_\ell(E)=(2ik)^{-1}(e^{2i\delta_\ell(E)}-1) \tag{112a}$$

$$f_\ell(E)=k^{-1}e^{i\delta_\ell(E)}\sin\delta_\ell(E) \tag{112b}$$

$$f_\ell(E)=k^{-1}(\cot\delta_\ell(E)-i)^{-1} \tag{112c}$$

where $k=\sqrt{E}$. In the rest of this section k will always denote $\sqrt{E}$. Notice that (112b) implies that

$$\operatorname{Im} f_\ell(E)=k|f_\ell(E)|^2 \tag{113}$$

This is often called **partial wave unitarity** because it is a direct translation of the unitarity of S. (110), (111), and (113) yield a new proof of the unitarity relation (97c).

The most important tool in the scattering theory for central potentials is the connection between phase shifts and the time-independent radial Schrödinger equation given by:

Theorem XI.53 Let V be central and piecewise continuous as a function of r on $[0,\infty)$. Suppose that $\int_0^1 r|V(r)|\,dr$ and $\int_1^\infty |V(r)|\,dr$ are finite. Fix $E>0$ and a nonnegative integer ℓ. Then there exists a unique function $\varphi_{\ell,E}(r)$ on $(0,\infty)$ that is C^1 and piecewise C^2 and which satisfies the equation

$$-\varphi''(r)+V_\ell(r)\varphi(r)=E\varphi(r) \tag{114}$$

where

$$V_\ell(r)=V(r)+\ell(\ell+1)r^{-2}$$

together with the boundary conditions

$$\lim_{r\to0}\varphi_{\ell,E}(r)=0,\qquad \lim_{r\to0}r^{-\ell-1}\varphi_{\ell,E}(r)=1$$

Further, there exists a constant c so that

$$\lim_{r\to\infty}[c\varphi_{\ell,E}(r)-\sin(kr-\tfrac{1}{2}\pi\ell+\delta_\ell(E))]=0 \tag{115}$$

where $\delta_\ell(E)$ is the scattering phase shift.

Proof One part of the proof involves applying the theory of ordinary differential equations to study (114). We shall quote several results of this study without proof. Later, in Section E, we shall prove these results in the case $\ell=0$. For proofs of the general ℓ results, see the references in the Notes. Although the second boundary condition implies the first, we write down both to emphasize the parallel to a second-order equation with $\varphi(x_0)=a$ and $\varphi'(x_0)=b$ as boundary conditions.

First suppose that $V\in C_0^\infty(\mathbb{R}^3)$ and that V is central. Fix a direction $\mathbf{e}$ and let $\varphi(\mathbf{x},k\mathbf{e})$ be the Lippmann–Schwinger wave function constructed in the proof of Theorem XI.41. Then

$$\varphi(x,ke)=e^{ike\cdot x}-\frac{1}{4\pi}\int\frac{e^{ik|x-y|}}{|x-y|}V(y)\varphi(y,ke)\,dy \tag{116}$$

Let $g\in C_0^\infty$ and let $h=(-\Delta-E)g$. Then

$$\int h(x)\varphi(x,ke)\,dx=-\frac{1}{4\pi}\iint h(x)\frac{e^{ik|x-y|}}{|x-y|}V(y)\varphi(y,ke)\,dy\,dx \tag{117}$$

where we have used the fact that $(-\Delta-E)e^{ike\cdot x}=0$ in distributional sense to eliminate the first term in (116). Since $|V|^{1/2}\varphi\in L^2$ and V and h are in C_0^∞, we can interchange the order of integration on the right-hand side of (117) and use

$$\int[(-\Delta-E)g](x)\frac{e^{ik|x-y|}}{4\pi|x-y|}\,d^3x=g(y)$$

to conclude that $(-\Delta-E)\varphi(x,ke)=-V(x)\varphi(x,ke)$ in distributional sense. By the elliptic regularity theorem (Theorem IX.26), we conclude that $\varphi(x,ke)$ is C^∞ in x and obeys the partial differential equation $(-\Delta+V)\varphi=E\varphi$ in the classical sense. Choose spherical coordinates $\langle r,\theta,\eta\rangle$ where θ is the angle between r and e. Then φ is independent of the azimuthal angle η. Let

$$\tilde\varphi_{\ell,E}(r)=\frac{r}{2}\int_0^\pi\varphi(r,\theta;ke)P_\ell(\cos\theta)\sin\theta\,d\theta$$

Then $\tilde\varphi_{\ell,E}$ obeys (114) and the first boundary condition. The theory of ordinary differential equations tells us that every solution of (114) obeying the first boundary condition is a multiple of the unique solution obeying both boundary conditions. If $\ell\neq0$, so that V_ℓ is singular at $r=0$, this fact is not as easy as in the case $\ell=0$ where we can appeal to Section V.6.A.

The proof of the theorem in case $V\in C_0^\infty$ is thus reduced to proving (115) with $\tilde\varphi$ replacing φ. In (116) fix $x\cdot e/|x|$ and let $|x|\to\infty$. Using the

definition of $T(\mathbf{k}, \mathbf{k}')$ and the fact that $V\varphi$ has compact support, it is easy to show that (Problem 78):

$$\lim_{\substack{|x|\to\infty \\ x\cdot e = |x|\cos\theta_0}} \left(\int \frac{e^{ik|x-y|}}{|x-y|} V(y)\varphi(y, ke)\, dy\right) e^{-ik|x|}|x| = (2\pi)^3 T(ke', ke) \tag{118}$$

where e' is chosen with $e \cdot e' = \cos\theta_0$. Moreover, the limit is uniform in θ_0. (105), (110b), and the definition of f imply that

$$\frac{1}{2}\int_0^\pi P_\ell(\cos\theta)\left[T(ke', ke)\Big|_{e\cdot e' = \cos\theta}\right]\sin\theta\, d\theta = -\frac{1}{2\pi^2} f_\ell(E)$$

By (116) and the uniformity of the limit in (118), we have

$$\lim_{r\to\infty} [\tilde{\varphi}(r) - e^{i\pi\ell/2} r j_\ell(kr) - f_\ell(E) e^{ikr}] = 0 \tag{119}$$

Here $j_\ell(kr)$ is the spherical Bessel function defined in the first appendix to this section. By Theorem XI.64, $yj_\ell(y) - \sin(y - \pi\ell/2) \to 0$ as $y \to \infty$ and moreover $f_\ell(E) = (e^{2i\delta_\ell} - 1)/2ik$. Thus

$$\lim_{r\to\infty} [2ik\tilde{\varphi}(r) - (e^{ikr} - e^{-ikr}e^{i\pi\ell}) - (e^{2i\delta_\ell} - 1)e^{ikr}] = 0$$

or

$$\lim_{r\to\infty} [ke^{-i\pi\ell/2}e^{-i\delta_\ell}\tilde{\varphi}(r) - \sin(kr - \tfrac{1}{2}\ell\pi + \delta_\ell)] = 0$$

This proves the theorem when $V \in C_0^\infty$. We approximate general V by $V_n \in C_0^\infty$. By Theorem XI.31 and Problem 28, as $V_n \to V$, the corresponding S-matrices converge, so the corresponding values of δ_ℓ converge. On the other hand, the method of Section E shows that the shifts of the phase of the solution of (114) converge. ∎

Thus δ_ℓ represents the shift in the phase of the solution of the radial Schrödinger equation regular at $r = 0$ relative to $j_\ell(kr)$, the solution when $V = 0$. In the above theorem we can drop the smoothness assumption on V if we replace the differential equation (114) by the integral equation (125). It is possible to prove (115) by developing a scattering theory directly for the Schrödinger operators on a fixed angular momentum subspace. This is discussed in Appendix 3.

D. The variable phase equation

In Section C we proved that the phase shift was connected to the radial Schrödinger equation. This connection suggests a great many additional results. For example, fix V obeying the conditions of Theorem XI.53. Suppose we make V more negative somewhere. Then for each fixed k, the solutions of $-\varphi'' + V_\ell\varphi = k^2\varphi$ oscillate more rapidly in the region where V has been made more negative. Thus we expect that the phase shift should be larger. We thus see that one expects that $\delta \geq \tilde{\delta}$ if $V \leq \tilde{V}$. It turns out to be difficult to prove this directly because of the π ambiguity in δ. For this reason, it is useful to develop additional tools for studying the phase shift. We develop two different methods in this subsection and the next. Both depend ultimately on Theorem XI.53.

Theorem XI.54 Let V obey the hypotheses of Theorem XI.53. Then, for each $k > 0$, there exists a unique solution of the equation

$$d'(r) = -\frac{1}{k} V(r)\sin^2(kr + d(r)), \qquad r \in (0, \infty) \tag{120}$$

satisfying the boundary condition $\overline{\lim}_{r\to 0} r^{-1}|d(r)| < \infty$. Moreover, the solution satisfies

$$\lim_{r\to\infty} d(r) = \delta_{\ell=0}(k^2) \tag{121}$$

where $\delta_{\ell=0}(k^2)$ is the s-wave phase shift for V, $\delta_0(k^2)$. Equation (120) is called the **variable phase equation**. We emphasize that $d(r)$ is k-dependent.

Proof The existence of solutions with the right boundary conditions follows from the contraction mapping theorem according to the pattern discussed in Section V.6.A. We leave the proof to Problem 79.

Fix ρ in $(0, \infty)$ and let V^ρ be defined by

$$V^\rho(r) = \begin{cases} V(r), & r \leq \rho \\ 0, & r > \rho \end{cases}$$

Let δ^ρ be the phase shift for V^ρ at fixed energy k^2. Since $V^\rho \to V$ in the norm given by (61), $\delta^\rho \to \delta$ as $\rho \to \infty$ (modulo π). We shall show that the function $\rho \mapsto \delta^\rho$ obeys the differential equation and the boundary condition at 0. This will allow us to conclude that (121) holds modulo π. We leave the question of resolving the modulo π ambiguity to Problem 80.

Let φ solve (114) for $\ell = 0$ and satisfy $\lim_{r\to 0} r^{-1}\varphi(r) = 1$. Let φ^ρ be the analogous function for V^ρ. Clearly,

$$\varphi^\rho(r) = \begin{cases} \varphi(r), & r \le \rho \\ \alpha \sin(kr + \beta), & r \ge \rho \end{cases}$$

for suitable α and β. By Theorem XI.53, $\beta = \delta^\rho$. The requirement that φ^ρ be C^1 implies

$$k \cot(k\rho + \delta^\rho) = \varphi'(\rho)/\varphi(\rho) \tag{122}$$

Using (122) and the differential equation (114), it is easy to prove that (Problem 81):

$$\frac{d\delta^\rho}{d\rho} = -\frac{1}{k} V(\rho)\sin^2(k\rho + \delta^\rho) \tag{123}$$

Moreover, by (122), $\lim_{\rho\to 0} \cot(k\rho + \delta^\rho) = \infty$. We resolve the π ambiguity in δ^ρ as defined in (122) by requiring $\lim_{\rho\to 0} \delta^\rho = 0$, and that δ^ρ be C^1. Finally, by (122), $\lim_{\rho\to 0} k\rho \cot(k\rho + \delta^\rho) = 1$ or

$$\lim_{\rho\to 0} (k\rho)^{-1}(k\rho + \delta^\rho) = 1$$

so, $\lim_{\rho\to 0} \rho^{-1}\delta^\rho = 0$. Thus by the uniqueness of solutions to equation (120), $\delta^\rho = d(\rho)$. ∎

Corollary 1 $\delta_0(E)$ may be chosen continuous in E for all E.

This is a corollary of part of the proof contained in Problem 80.

Corollary 2 If $\delta_0(E)$ is chosen to be continuous with $\lim_{E\to\infty} \delta_0(E) = 0$, then the phase shifts for $-\Delta + \lambda V$ are continuous in λ and go to zero as $\lambda \to 0$.

The proof is left to Problem 82.

Corollary 3 δ_0 is positive for an everywhere negative potential ($V(r) \le 0$ all r) and negative for an everywhere positive potential.

Proof $\delta_0(k^2) = -k^{-1}\int_0^\infty V(r)\sin^2(kr + d(r))\,dr$ by (120) and (121). This is clearly positive (respectively, negative) if $V \le 0$ (respectively, $V \ge 0$). ∎

Corollary 4 If $V \le \tilde{V}$, the s-wave phase shifts for V are greater than or equal to those for $\tilde{V}$.

Proof Fix $k > 0$. Suppose first that $V = \tilde{V}$ in $(0, \rho_0)$ and that $V < \tilde{V}$ in (ρ_0, ∞). Let $d(\rho)$, $\tilde{d}(\rho)$ be the corresponding solutions of the variable phase equation, (120). Then $d(\rho_0) = \tilde{d}(\rho_0)$ and $d'(\rho_0) = \tilde{d}'(\rho_0)$ by (120), so $d(\rho) > \tilde{d}(\rho)$ for ρ near and larger than ρ_0. If $\tilde{d}$ were ever larger than d, there would be $\rho_1 > \rho_0$ with $d(\rho_1) = \tilde{d}(\rho_1)$ and $\tilde{d}'(\rho_1) \ge d'(\rho_1)$. This is inconsistent with (120) and $V < \tilde{V}$ in (ρ_0, ∞). Thus $d \ge \tilde{d}$ for all ρ and, by (121), $\delta \ge \tilde{\delta}$. For the general case, one uses a simple limiting argument. ∎

The low energy behavior of $\delta_0(E)$ is of especial interest. It may be studied by a method related to the variable phase method.

Theorem XI.55 Let $V \in C_0^\infty(\mathbb{R}^3)$ be a central potential and let u be the solution of $-u''(r) + V(r)u(r) = 0$ with boundary conditions $u(0) = 0$, $u'(0) = 1$. Then:

(a) If $\lim_{r\to\infty} u'(r) \neq 0$ and $u(r)$ has m zeros different from $r = 0$, then

$$\lim_{k\to 0} \delta_0(k^2) = m\pi \qquad \text{and} \qquad \lim_{k\to 0} \frac{\delta_0(k^2) - m\pi}{k} = \lim_{r\to\infty} \frac{u(r) - ru'(r)}{u'(r)}$$

(b) If $\lim_{r\to\infty} u'(r) = 0$ and $u(r)$ has m zeros different from $r = 0$, then

$$\lim_{k\to 0} \delta_0(k^2) = (m + \tfrac{1}{2})\pi$$

Proof We use equations (122) and (123). Choose R so that all the zeros of u lie in $(0, R)$ and so that $V(r) = 0$ if $r > R$. In particular, $u(r) = a(r - R) + b$ for $r > R$. Since $u(r)$ has no zeros in (R, ∞), we have that $a/b = u'(R)/u(R) \ge 0$. Let $\varphi_E(r)$ denote the solution of (114) satisfying $\varphi_E(0) = 0$ and $\varphi_E'(0) = 1$. Writing the differential equation as an integral equation, one sees that $\varphi_E(r) \to \varphi_0(r)$ as $E \to 0$, uniformly on $[0, R + 1]$. In particular, for some E_0, $\varphi_E(r)$ has m zeros in $[0, R)$ if $E < E_0$ and $\varphi_E(R)^{-1}\varphi_E'(R) \to a/b$. By the proof of Theorem XI.54, $\delta_0(E)$ is determined by

$$k \cot(k\rho + d(\rho, k)) = \varphi_E'(\rho)/\varphi_E(\rho) \tag{122}$$

$d(\cdot, k)$ continuous, $d(0, k) = 0$, $d(R, k) = \delta_0(k^2)$. Clearly at each point ρ that $\varphi_E(\rho)$ vanishes, $k\rho + d(\rho, k)$ must take one of the values $0, \pm\pi, \ldots$. Moreover, by (123), at each such point, $(\partial/\partial\rho)d(\rho, k) = 0$, so that $(\partial/\partial\rho)(k\rho + d(\rho, k)) > 0$. Thus

$$m\pi \le kR + d(R, k) < (m + 1)\pi \tag{124}$$

if $k < E_0$. $d(R, k) = \delta_0(k)$ is thus uniquely determined by (122) and (124). If $u'(R) = \lim_{r\to\infty} u(r) \neq 0$, then for all small E, $\varphi_E'(R)/\varphi_E(R) \ge \frac{1}{2}u'(R)/u(R) > 0$

so, by (122), $\cot(kR + d(R, k)) \to \infty$ as $k \to 0$. This is only consistent with (124) if $kR + d(k, R) \to m\pi$. On the other hand, by the integral equation, $\varphi'_E(R)$ is a C^∞ function of k^2 at $k = 0$, so if $u'(R) = 0$, then $\varphi'_E(R)$ vanishes as k^2 at $k = 0$. Thus, in that case, $\cot(kR + d(R, k)) \to 0$ by (122), so $kR + d(R, k) \to (m + \frac{1}{2})\pi$. The remaining statement in (a) is left to the reader (Problem 83). ∎

It is possible to considerably weaken the hypotheses on V in the preceding theorem.

Definition The quantity

$$\lim_{r\to\infty} \frac{u(r) - ru'(r)}{u'(r)} = \lim_{k\to 0} \frac{\delta_0(k) - \delta_0(0)}{k}$$

is called the **scattering length**. If $\lim_{r\to\infty} u'(r) = 0$, we say the scattering length is infinite.

The scattering length a is a natural scattering parameter because, by (112), $\lim_{E\to 0} f_{\ell=0}(E) = a$. Moreover, it can be shown under many circumstances that $\sum_{\ell\geq 1} k^{-2} \sin^2 \delta_\ell(k^2) \to 0$ as $k \to 0$ so that $\lim_{E\to 0} \sigma_{\text{tot}}(E) = 4\pi a^2$ by (111).

E. Jost functions and Levinson's theorem

Theorem XI.53 relates the phase shift to solutions of the radial Schrödinger equation, at least when V is regular. To discuss general V, and also in order to discuss systematically the solutions of (114), it is useful to rewrite the Schrödinger equation with boundary conditions as an integral equation. As a dividend of our development of the integral equation approach, we shall relate the number of spherically symmetric eigenfunctions to the s-wave phase shift. We discuss only the $\ell = 0$ case. References for the general case can be found in the Notes.

Definition The **Schrödinger integral equation with regular boundary conditions at 0**, or, for short the **regular equation** is

$$f(x) = x + \int_0^x (x - y)[V(y) - k^2]f(y)\, dy \tag{125}$$

Definition Let $k \neq 0$. The **Schrödinger integral equation with Jost boundary conditions at ∞**, or, for short the **Jost equation** is

$$f(x) = e^{-ikx} - \int_x^\infty \frac{\sin k(x - y)}{k} V(y)f(y)\, dy \tag{126}$$

When V is sufficiently regular, for example if V is continuous, (125) and (126) are equivalent to the Schrödinger differential equation (114) with appropriate boundary conditions. There is a systematic method known as the method of variation of parameters which can be used to rewrite second-order differential equations with boundary conditions as integral equations (see Appendix 2).

Theorem XI.56 Suppose that V is a measurable function obeying $N(x) \equiv \int_0^x y|V(y)|\, dy < \infty$ for each $x > 0$. Then, for each $k \in \mathbb{C}$, the regular equation (125) has a unique solution $\varphi(x, k)$ that is locally bounded on $(0, \infty)$ and obeys $\overline{\lim}_{x\to 0} |x^{-1}\varphi(x)| < \infty$. Moreover, $\varphi(x, k)$ is continuously differentiable in x on $[0, \infty)$ with $\varphi(0, k) = 0$, $\varphi'(0, k) = 1$ and, for each fixed x, $\varphi(x, k)$ and $\varphi'(x, k)$ are entire functions of k obeying

$$|\varphi(x, k)| \leq x \exp[N(x) + \tfrac{1}{2}|k|^2x^2]$$
$$|\varphi'(x, k)| \leq \exp[N(x) + \tfrac{1}{2}|k|^2x^2]$$

In addition $\overline{\varphi(x, k)} = \varphi(x, \bar{k})$. φ is called the **regular solution**.

Proof Let $\psi(x) = f(x)/x$ so that to solve (125), we seek ψ obeying

$$\psi(x) = 1 + \int_0^x K(x, y)\psi(y)\, dy \tag{127}$$

where

$$K(x, y) = y\left(1 - \frac{y}{x}\right)(V(y) - k^2)$$

By iterating (127), we obtain a formal series

$$\psi(x) = \sum_{n=0}^\infty \psi_n(x) \tag{128}$$

where

$$\psi_0(x) = 1, \qquad \psi_n(x) = \int_0^x K(x, y)\psi_{n-1}(y)\, dy$$

We shall prove inductively that

$$|\psi_n(x)| \le (n!)^{-1} P(x)^n \tag{129}$$

where

$$P(x) = N(x) + \tfrac{1}{2}|k|^2 x^2$$

(129) certainly holds if $n = 0$. If $0 \le y \le x$, then

$$|K(x, y)| \le y(|V(y)| + |k^2|)$$

so if ψ_n obeys (129), then

$$\begin{aligned} |\psi_{n+1}(x)| &\le \int_0^x y(|V(y)| + |k|^2)(n!)^{-1} P(y)^n \, dy \\ &= (n!)^{-1} \int_0^x (P(y))^n \frac{dP}{dy} \, dy \\ &= [(n+1)!]^{-1} (P(x))^{n+1} \end{aligned}$$

so (129) holds by induction.

We conclude that (128) converges uniformly on compacts in x and k. Since each $\psi_n(x)$ is analytic in k (it is a polynomial!), the limiting function is analytic in k. ψ obeys (127), so φ obey (125). The bound on φ follows from (129). The analyticity of φ' in k and the bound on φ' follow from the formula

$$\varphi'(x, k) = 1 - \int_0^x y(V(y) - k^2)\psi(y, k) \, dy$$

and the bound (129). Uniqueness is left to the reader (Problem 84). ∎

Theorem XI.57 Suppose that V is a measurable function obeying $\int_x^\infty |V(y)| \, dy < \infty$ for each $x > 0$. Define $Q_k(x)$ by

$$Q_k(x) = \int_x^\infty (1 + |k|y)^{-1} 4y |V(y)| e^{(\operatorname{Im} k + |\operatorname{Im} k|)y} \, dy$$

Then:

(a) For each $k \in \mathbb{C}$, with $\operatorname{Im} k \le 0$, and $k \ne 0$, the Jost equation (126) has a unique solution $\eta(x, k)$ obeying $\lim_{x\to\infty} |e^{ikx}\eta(x, k)| < \infty$. Moreover, $\eta(x, k)$ is continuously differentiable in x on $[0, \infty)$ with $\lim_{x\to\infty} e^{ikx}\eta(x, k) = 1$ and $\lim_{x\to\infty} e^{ikx}\eta'(x, k) = -ik$. For each fixed x, $\eta(x, k)$ and $\eta'(x, k)$ are functions analytic in $\{k \mid \operatorname{Im} k < 0\}$, continuous in $\{k \mid \operatorname{Im} k \le 0; k \ne 0\}$, obeying

$$|\eta(x, k) - e^{-ikx}| \le e^{(\operatorname{Im} k)x} |e^{Q_k(x)} - 1| \tag{130a}$$

$$|\eta'(x, k) + ike^{-ikx}| \le e^{(\operatorname{Im} k)x} e^{Q_k(x)} \int_x^\infty |V(y)| \, dy \tag{130b}$$

(b) If, in addition, $\int_0^\infty x|V(x)| \, dx < \infty$, then $\eta(x, k)$ may be extended to $k = 0$ in such a way that $\eta(x, k)$ is continuous on $\{k \mid \operatorname{Im} k \le 0\}$. Moreover, (130) continues to hold.

(c) If, in addition, $\int_x^\infty e^{my}|V(y)| \, dy < \infty$, then $\eta(x, k)$ can be extended, for each x, to a function analytic in $\{k \mid \operatorname{Im} k < \frac{1}{2}m\}$. Moreover, (130) continues to hold.

In each case, η obeys $\overline{\eta(x, k)} = \eta(x, -\bar{k})$. η is called the **Jost solution.**

Proof The idea is very similar to the proof of Theorem XI.56, so we only sketch the proof leaving the details to the reader (Problem 85). (126) is formally solved by the series

$$\eta(x, k) = \sum_{n=0}^\infty \eta_n(x, k)$$

where $\eta_0(x, k) = e^{-ikx}$ and

$$\eta_n(x, k) = \int_x^\infty k^{-1}[\sin k(y - x)]V(y)\eta_{n-1}(y, k) \, dy$$

From the bound

$$\frac{|\sin k(x - y)|}{|k|} \le \frac{4y}{1 + |k|y} \exp[|\operatorname{Im} k|y + (\operatorname{Im} k)x], \qquad y \ge x \ge 0$$

one obtains by induction

$$|\eta_n(x, k)| \le (n!)^{-1} Q_k(x)^n$$

If we interpret $k^{-1} \sin k(x - y)$ as $(x - y)$ when $k = 0$, then these bounds continue to hold when $k = 0$. Each $\eta_n(x, k)$ is easily seen to be analytic in the interior of the region where $Q_k(1) < \infty$ and continuous on the boundary. The assertions of the theorem are proven by summing the series. ∎

We now define the Jost function, which we shall see is intimately connected to the scattering amplitude.

Theorem XI.58 Let V obey

$$\int_0^x |y|\,|V(y)|\,dy + \int_x^\infty |V(y)|\,dy < \infty$$

for each x. Then:

(a) $\eta(k) \equiv \eta(x, k)\varphi'(x, k) - \eta'(x, k)\varphi(x, k)$ is independent of x. $\eta(k)$ is called the **Jost function**.

(b) $\eta(k)$ is analytic in $\{k \mid \operatorname{Im} k < 0\}$ and continuous in $\{k \mid \operatorname{Im} k \leq 0;\ k \neq 0\}$. If V obeys $\int_1^\infty e^{my}|V(y)|\,dy < \infty$, for some $m > 0$, then $\eta(k)$ is analytic in $\{k \mid \operatorname{Im} k < \frac{1}{2}m\}$.

(c) If k is real and nonzero, then $\eta(k) \neq 0$, $\eta(-k) = \overline{\eta(k)}$ and

$$\frac{\eta(k)}{\eta(-k)} = e^{2i\delta_0(k)}$$

where $\delta_0(k)$ is the s-wave phase shift.

(d) All the zeros of $\eta(k)$ in $\{k \mid \operatorname{Im} k < 0\}$ are simple. They lie on the imaginary axis and k is a zero if and only if k^2 is an $\ell = 0$ bound state energy.

(e) $\lim_{\substack{k\to\infty \\ \operatorname{Im} k \leq 0}} \eta(k) = 1$.

Proof (a) First suppose that $V \in C_0^\infty(0, \infty)$. Then η and φ both obey the differential equation $-u'' + Vu = k^2u$ so $\eta\varphi' - \eta'\varphi$ is constant since it is the Wronskian of two solutions (an explicit computation shows that $(\eta\varphi' - \eta'\varphi)' = 0$). If V is an arbitrary potential obeying the hypothesis, we can find $V_n \in C_0^\infty$, so that $\int_0^1 y|V_n - V|\,dy + \int_1^\infty |V_n - V|\,dy \to 0$ as $n \to \infty$. By the construction of φ and η, we conclude that $\varphi_n \to \varphi$, $\varphi_n' \to \varphi'$, $\eta_n \to \eta$, $\eta_n' \to \eta'$ pointwise, so (a) holds in general. For the proof of our assertion that η is called the Jost function, see the Notes.

(b) This follows from the analyticity properties of φ, φ', η, η' stated in Theorems XI.56 and XI.57.

(c) Since $\overline{\varphi(x, k)} = \varphi(x, k) = \varphi(x, -k)$ and $\overline{\eta(x, k)} = \eta(x, -k)$ when k is real, we conclude that $\eta(-k) = \overline{\eta(k)}$. Next we claim that

$$\varphi(x, k) = (2ik)^{-1}\{\eta(k)\eta(x, -k) - \eta(-k)\eta(x, k)\} \tag{131}$$

We shall prove (131) and the basic relation $\eta(k)/\eta(-k) = e^{2i\delta_0}$ for $V \in C_0^\infty(0, \infty)$. The general case then follows by a limiting argument as in the proof of (a). Suppose that supp $V \subset [a, b]$, $0 < a < b < \infty$. Then $\varphi(\cdot, k)$, $\eta(\cdot, k)$, and $\eta(\cdot, -k)$ are all solutions of $-u'' + Vu = k^2u$. Moreover, for $x > b$, $\eta_\pm(x) \equiv \eta(x, \pm k) = e^{\pm ikx}$, so $\eta_\pm$ are linearly independent and their Wronskian $W(\eta_+, \eta_-) = \eta_+\eta_-' - \eta_-\eta_+'$ is $2ik$. Thus

$$\varphi = W(\eta_+, \eta_-)^{-1}[W(\eta_+, \varphi)\eta_- - W(\eta_-, \varphi)\eta_+]$$

which is (131).

(131), $\eta(k) = \overline{\eta(-k)}$, and the fact that φ is not identically zero imply that $\eta(k) \neq 0$. Moreover, since $\eta_\pm(x) = e^{\pm ikx}$ for $x > b$, we see that

$$\varphi(x) = k^{-1}|\eta(k)|\,\sin(kx + d(k))$$

for $x > b$ if $\eta(k) = |\eta(k)|e^{id(k)}$. By Theorem XI.53, we conclude that $d(k) = \delta_0(k) \pmod{2\pi}$.

(d) We first claim that $(-\Delta + V - k^2)(x^{-1}\varphi(x, k)) = 0$ where $-\Delta$ is to be interpreted in distributional sense. For this holds if $V \in C_0^\infty(0, \infty)$ and so for general V by a limiting argument. If $\eta(k) = 0$, then φ is a constant multiple of η and so in L^2 at infinity. Thus k is purely imaginary and k^2 is an eigenvalue.

Conversely, suppose that $V \in C_0^\infty$ and that k^2 is an $\ell = 0$ eigenvalue of $-\Delta + V$. Since V falls off exponentially, η is an entire function, so (131) holds for all k. Then, by this analytic continuation of (131), $\eta(k) = 0$. By a limiting argument, this extends to all V.

Finally, we must show that the zeros of η are simple. We first note that if $u = x^{-1}\varphi$ and $v = x^{-1}\,\partial\varphi/\partial k$, then

$$(-\Delta + V - k^2)u = 0 \tag{132a}$$

$$(-\Delta + V - k^2)v = 2ku \tag{132b}$$

in distributional sense. Moreover, if $\eta(k_0) = (\partial\eta/\partial k)(k_0) = 0$, then one can show that

$$\frac{\partial\varphi}{\partial k} = c_1\eta + c_2\frac{\partial\eta}{\partial k}$$

so $v \in L^2$. But if $u, v \in L^2$, then (132) is inconsistent with $u \neq 0$ since

$$2k\|u\|^2 = (u, (-\Delta + V - k^2)v) = 0$$

Thus, if $\eta(k_0) = 0$, then $\partial\eta/\partial k \neq 0$ at k_0, so the zeros of η are simple.

(e) By (130a) and $\eta(k) = \eta(0, k)$,

$$|\eta(k) - 1| \leq |\exp Q_k(0) - 1|$$

if $\operatorname{Im} k \leq 0$. Thus it suffices to prove that

$$\lim_{k\to\infty} \int_0^\infty \frac{y|V(y)|}{1 + |k|y} = 0$$

and this follows from the monotone convergence theorem. ∎

One of the more spectacular consequences of the machinery of Jost functions is:

Theorem XI.59 (Levinson's theorem) Let V obey $\int_0^\infty x|V(x)|\,dx < \infty$ and let η be the Jost function and δ_0 the s-wave phase shift normalized by $\lim_{k\to\infty} \delta_0(k^2) = 0$. Then

$$\delta_0(0) = \begin{cases} n_0\pi, & \text{if } \eta(0) \neq 0 \\ (n_0 + \tfrac{1}{2})\pi, & \text{if } \eta(0) = 0 \end{cases}$$

where n_0 is the number of eigenvalues with spherically symmetric eigenfunctions for $-\Delta + V$.

Proof We consider the case $\eta(0) \neq 0$. The case $\eta(0) = 0$ is left to the problems. By (131), all $\ell = 0$ eigenfunctions have $k^2 < 0$, so by Theorem XI.58d, n_0 is the number of zeros of $\eta(k)$ in the lower half-plane. Let $0 < \theta < \frac{1}{2}\pi$. Pick R_0, so that $|\eta(k) - 1| < 2\sin(\frac{1}{2}\theta)$ for $|k| \geq R_0$, $\operatorname{Im} k \leq 0$. By Theorem XI.58e, such an R_0 exists. Consider the integral of η'/η around the contour $C = C_1 \cup C_2$ in Figure XI.10. The poles of η'/η are at the zeros of η and since

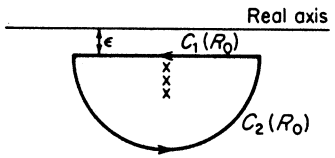


FIGURE XI.10 A contour for Levinson's theorem.

these zeros are simple, the residues are equal to 1. Thus

$$n_0 = (2\pi i)^{-1} \int_C \frac{\eta'}{\eta}\, dz$$

Now $i^{-1}\eta'/\eta = d(\arg \eta)/dz$, so in the limit as $\varepsilon \to 0$, the contribution of C_1 is $\pi^{-1}(\delta_0(0) - \delta_0(R_0^2))$. Since $|\arg \eta| < \theta$ on all of $C_2(R_0)$ by the choice of R_0, we conclude that

$$|\pi^{-1}[\delta_0(0) - \delta_0(R_0^2)] - n_0| \leq 2\theta$$

Taking $R_0 \to \infty$, $\theta \to 0$, we see that $\delta_0(0) = n_0\pi$. ∎

We saw in Section 7 that the poles in the upper half-plane of the forward scattering amplitude can occur only at points k where k^2 is an eigenvalue of $-\Delta + V$. The formula

$$f_{\ell=0}(k^2) = 2ik^{-1}(\eta(k) - \eta(-k))/\eta(-k)$$

which follows from Theorem XI.58c together with the fact that the only zeros of $\eta(-k)$ are at points where k^2 is an eigenvalue, suggests that the poles of $f_{\ell=0}(k^2)$ in the upper half-plane are also connected only to bound states. This is false. In the first place, for general potentials the analyticity domains of $\eta(k)$ and $\eta(-k)$ are disjoint and there may be no continuation for $f_{\ell=0}$. Moreover, it can happen that $\eta(k)$ has a meromorphic continuation to the upper half-plane with poles at certain points. These poles will produce poles in $f_{\ell=0}$ which do not correspond to bound states. This phenomenon will be discussed further in the next subsection.

F. Analyticity of the partial wave amplitude for generalized Yukawa potentials

In Section 7 we saw that the full scattering amplitude $f(E, \cos\theta)$ has analyticity properties in E at $\cos\theta = 1$ under rather general circumstances. Analyticity at $\theta \neq 0$ required some exponential falloff. Not surprisingly then, analyticity properties for $f_0(k)$, the s-wave scattering amplitude, requires exponential falloff. From the results of part E, and the formula $ss_0(k^2) = \eta(k)/\eta(-k)$ and $f_0(k^2) = (2ik)^{-1}[s_0(k^2) - 1]$, we see that:

Theorem XI.60 If $\int_1^\infty e^{my}|V(y)|\,dy + \int_0^1 y|V(y)|\,dy < \infty$, then the s-wave partial wave amplitude is real analytic on $(0, \infty)$ and has a meromorphic continuation from the upper edge of the real axis into the parabolic

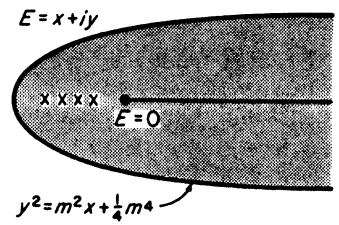


FIGURE XI.11 Analyticity region for $f_0(E)$, general case.

region, $\{E \,|\, |E| - \operatorname{Re} E \leq \frac{1}{2}m^2, E \text{ not a positive real}\}$ (see Figure XI.11), with poles precisely at the energies of bound states in the region $E > -\frac{1}{4}m^2$.

Proof Let $G(k) = \eta(k)/\eta(-k)$. Then G is analytic in the region $|\operatorname{Im} k| \leq \frac{1}{2}m$. In the region $\operatorname{Im} k > 0$, $G(k)$ can have poles only when $\eta(-k) = 0$. If $\eta(-k) = 0$, $\eta(k) \neq 0$ by the analytic continuation of (131). Thus G has poles precisely at zeros of $\eta(-k)$. The theorem now follows from the formula $f_0(E) = (2i\sqrt{E})^{-1}[G(\sqrt{E}) - 1]$. ∎

For the generalized Yukawa potentials defined in Section 7, we can say much more (μ_0 is the constant occurring in the definition of generalized Yukawa potentials):

Theorem XI.61 Let $f_0(E)$ be the s-wave scattering amplitude for a generalized Yukawa potential. Then there is a function $F(E)$, meromorphic in $D = \mathbb{C}\backslash([0, \infty) \cup (-\infty, -(\frac{1}{2}\mu_0)^2])$, so that for $E \in (0, \infty)$

$$f_0(E) = \lim_{\varepsilon \downarrow 0} F(E + i\varepsilon)$$

The only poles of F *in* D occur on the negative axis at bound state energies, and there is a pole at each such energy in $(-(\frac{1}{2}\mu_0)^2, 0)$. Moreover, $f_0(E)$ is real analytic on $(0, \infty)$.

Before turning to the proof of Theorem XI.61, we make a series of remarks, one of which explains the reason for emphasizing that it is only the poles *in* D that are described in the theorem. First, one can prove that f is analytic in $\mathbb{C}\backslash([0, \infty) \cup (-\infty, -\mu_0^2])$. Secondly, we shall actually prove more than is stated in the theorem. We shall show that the function $G(k)$ defined by $G(k) = F(k^2)$ for $\operatorname{Im} k > 0$ has a meromorphic continuation to $\mathbb{C}\backslash([\frac{1}{2}i\mu_0, i\infty) \cup (-i\infty, -\frac{1}{2}i\mu_0])$—see Figure XI.12. As a result, the cut from 0

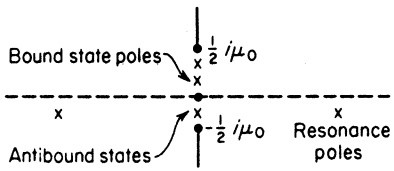


FIGURE XI.12 (a) Region for $G(-k)$, (b) analyticity region for $F(E)$.

to ∞ in $F(E)$ is due entirely to the use of the variable $E = k^2$, and one can continue onto a second sheet by continuing past this cut. Poles of $F_0(E)$ on the second sheet with $\operatorname{Im} E \neq 0$ (equivalently, poles of $G(k)$ at points with $\operatorname{Re} k \neq 0$, $\operatorname{Im} k < 0$) are called **resonance poles**—one can show that they correspond precisely to the resonances that will be discussed in Section XII.6 since the generalized Yukawa potentials are dilation analytic. Poles corresponding to $k \in (-\frac{1}{2}i\mu_0, 0)$ are called **antibound states**.

Since the cut in $[0, \infty)$ is due entirely to the use of the variable E instead of k, it is often called the **kinematical cut**. It is also called the **unitarity cut** since its discontinuity is given by the unitarity relation

$$F(E + i0) - F(E - i0) = 2 \operatorname{Im} f_0(E) = E^{1/2} |f_0(E)|^2$$

The cut in $(-\infty, -(\frac{1}{2}\mu_0)^2]$ is directly related to the potential in that its discontinuities can be computed directly from the potential by an iterative scheme (see the Notes). This cut is called the **dynamical cut**. The phrase **left-hand cut** and **right-hand cut** are sometimes used in place of dynamical cut and kinematical cut.

Finally, there is one subtle point. It can happen that the left-hand cut partly "degenerates into poles," that is, that $F(E)$ has a meromorphic continuation into a region including $(-a, -(\frac{1}{2}\mu_0)^2)$, $a > (\frac{1}{2}\mu_0)^2$, with poles in this region. The poles of $F(E)$ in this interval may not be connected with bound states; for this reason, they are often called **false poles**. In fact, there exist distinct generalized Yukawa potentials, V_1 and V_2, for which the corresponding s-wave partial wave amplitudes are equal but which are distinguished by the fact that all the poles of $F(E)$ are associated with bound states of $-\Delta + V_1$ while the leftmost pole of $F(E)$ is not associated with a bound state of $-\Delta + V_2$ but rather with its dynamical cut! This example is especially surprising because of Levinson's theorem which tells us that $F(E + i0)$ determines the number of bound states and so, one would assume, the number of bound state poles. The point is that if a bound state energy is not in $(-a, -(\frac{1}{2}\mu_0)^2)$, the pole which one would expect to be there can have a zero residue. Thus, while $-\Delta + V_1$ and $-\Delta + V_2$ have the same number of bound states of angular momentum zero, they have different numbers of "bound state poles."

Throughout the proof of Theorem XI.61, we shall suppose that V is of the form $V(x) = x^{-1}e^{-\mu_0 x}$. It is a simple exercise to extend the proof to generalized Yukawa potentials. The main idea is to use the analyticity of $V(x)$ in the region $\{x \mid \operatorname{Re} x > 0\}$ to extend the Jost function $\eta(k)$ in k. There is thus a close connection between these ideas and the dilation analytic ideas of Sections XII.6 and XIII.10. Our extension of $\eta(k)$ is in two steps:

Lemma 1 The function $\eta(x, k)$ which is defined initially on $\{\langle x, k\rangle \mid x \in (0, \infty), \operatorname{Im} k \leq 0\}$ can be extended to $\Omega = \{\langle x, k\rangle \mid \operatorname{Re} x > 0, \operatorname{Im} k \leq 0\}$ in such a way as to be a jointly analytic function of x and k in Ω^{int}, continuous in Ω. Moreover, in Ω, it obeys the differential equation

$$-\frac{d^2}{dx^2}\eta(x, k) + V(x)\eta(x, k) = k^2\eta(x, k)$$

and in the region $\Omega' = \{\langle x, k\rangle \in \Omega \,|\, |x| > 1\}$, it obeys the bound

$$|\eta(x, k) - e^{-ikx}| \leq e^{\mathrm{Im}(kx)}\{\exp[\mu_0^{-1}|k|^{-1}e^{-\mu_0 \mathrm{Re}\, x}] - 1\} \tag{133}$$

Proof We shall show that η can be extended to Ω' obeying (133). By the same method, one can extend η to the region $\{\langle x, k\rangle \in \Omega \,|\, |x| > \varepsilon\}$ and so to all of Ω. Since the differential equation is valid when x is real, it holds for all x by analytic continuation. Fix k with $\mathrm{Im}\, k \leq 0$. Define $\eta_n(x, k)$ inductively on Ω' by

$$\eta_0(x, k) = e^{-ikx}$$

$$\eta_n(x, k) = \int_0^\infty k^{-1}(\sin ky)V(y + x)\eta_{n-1}(y + x, k)\, dy$$

A change of variables shows that when x is real, $\eta_n(x, k)$ agrees with the function defined in the proof of Theorem XI.57. Moreover, we claim the following bound holds in Ω':

$$|\eta_n(x, k)| \leq (n!)^{-1}e^{\mathrm{Im}(kx)}(\mu_0|k|)^{-n}e^{-n\mu_0 \mathrm{Re}\, x} \tag{134}$$

(134) certainly holds when $n = 0$; and if it holds for some n, then

$$\begin{aligned}|\eta_{n+1}(x, k)| &\leq (n!)^{-1}(\mu_0|k|)^{-n} \\ &\quad \times \int_0^\infty |k|^{-1}e^{y|\mathrm{Im}\, k|}e^{-\mu_0(\mathrm{Re}\, x + y)(n+1)}e^{\mathrm{Im}(kx) + (\mathrm{Im}\, k)y}\, dy \\ &= [(n + 1)!]^{-1}(\mu_0|k|)^{-n-1}e^{-(n+1)\mu_0 \mathrm{Re}\, x}\end{aligned}$$

since $|\mathrm{Im}\, k| + \mathrm{Im}\, k = 0$ when $\mathrm{Im}\, k \leq 0$ and $(x + y)^{-1} \leq 1$ when $|x| > 1$, $\mathrm{Re}\, x > 0$, $y \in (0, \infty)$. This proves (134) inductively.

By (134), the integral defining η_n converges absolutely, so η_n is analytic in $(\Omega')^{\mathrm{int}}$. Since $\sum_n \eta_n$ converges absolutely by (134), the limit has the required analyticity and obeys the bound (133). ∎

Lemma 2 The Jost function $\eta(k)$ can be analytically continued to $\mathbb{C}\backslash[\frac{1}{2}i\mu_0, i\infty)$.

Proof Since we already know by Theorem XI.58 that $\eta(k)$ is analytic in $\{k \,|\, \mathrm{Im}\, k \leq \frac{1}{2}\mu_0\}$, we need only prove that $\eta(k)$ has an analytic continuation to every half-plane of the form $\{k \,|\, \mathrm{Im}(e^{-i\alpha}k) \leq 0\}$ for each $\alpha \in (-\frac{1}{2}\pi, \frac{1}{2}\pi)$. Fix such an α and define $\tilde{\eta}$ on $\{\langle y, k\rangle \,|\, y \in \mathbb{R}, \mathrm{Im}\, k \leq 0\}$ by

$$\tilde{\eta}(y, k) = \eta(e^{-i\alpha}y, k)$$

where $\eta(x, k)$ is continued to complex x by using Lemma 1. Then $\tilde{\eta}$ obeys the differential equation

$$\left(-\frac{d^2}{dy^2} + \tilde{V}(y)\right)\tilde{\eta}(y, k) = \tilde{k}^2\tilde{\eta}(y, k) \tag{135}$$

where $\tilde{V}(y) = e^{-2i\alpha}V(e^{-i\alpha}y)$ and $\tilde{k} = e^{-i\alpha}k$. Moreover, by (133),

$$|\tilde{\eta}(y, k) - e^{-ik_y}| \to 0 \tag{136}$$

as $y \to \infty$, so long as $\mathrm{Im}\, \tilde{k} \leq 0$, $\mathrm{Im}\, k \leq 0$. In the proof of Theorem XI.57, the reality of V was not used anywhere, so we know that (135) has a unique solution $\eta_1(y, \tilde{k})$ for $\{\langle y, k\rangle \,|\, y \in [0, \infty), \mathrm{Im}\, \tilde{k} \leq 0\}$ obeying (136). Thus $\tilde{\eta}(y, k)$ and $\eta_1(y, e^{-i\alpha}k)$ agree in the region $\{k \,|\, \mathrm{Im}\, k \leq 0, \mathrm{Im}(e^{-i\alpha}k) \leq 0\}$ so η_1 is an analytic continuation of $\tilde{\eta}$ to $\{k \,|\, \mathrm{Im}(e^{-i\alpha}k) \leq 0\}$. In particular, $\eta(k) = \tilde{\eta}(0, k)$ has a continuation to $\{k \,|\, \mathrm{Im}(ke^{-i\alpha}) \leq 0\}$. ∎

Proof of Theorem XI.61 Since $f_0(k^2) = (2ik)^{-1}[e^{2i\delta_0(k)} - 1]$, we need only prove the analyticity statements for $s_0(k) = e^{2i\delta_0(k)}$. But since $s_0(k) = \eta(k)/\eta(-k)$, we see that $s_0(k)$ is meromorphic in $D = \{k \,|\, k \notin [\frac{1}{2}i\mu_0, \infty) \cup (-\infty, -\frac{1}{2}i\mu_0]\}$ and the only poles in $D \cap \{k \,|\, \mathrm{Im}\, k > 0\}$ occur at points k_0 with $\eta(-k_0) = 0$. Moreover, as in the proof of Theorem XI.60, poles occur at all such k_0. ∎

G. The Kohn variational principle

In the discussion of the variable phase method, we saw that the scattering length, a, was an important parameter since, under some circumstances, $\lim_{E\to 0} \sigma_{\mathrm{tot}}(E) = 4\pi a^2$. Recall that the scattering length for potentials V with compact support was determined by finding a suitable normalized solution of $-\varphi'' + V\varphi = 0$, $\varphi(0) = 0$, with $\varphi(r) = r + a$ for r large. Consider real-valued functions, ψ, on $[0, \infty)$ of the form

$$\psi = \alpha r + \beta + g \tag{136a}$$

with g smooth, g, g', g'' falling off faster than any polynomial and $\psi(0) = 0$. Let Q be the set of such functions and let $\alpha(\psi)$, $\beta(\psi)$ be the constants in (136a).

For ψ, η in Q, we can define a natural object,

$$(\psi, h\eta) = \int_0^\infty \psi(r)(-\eta''(r) + V(r)\eta(r))\, dr$$

since $\bar{\psi}(-\eta'')$ is in L^1. However, it is false that $(\psi, h\eta)$ and $(\eta, h\psi)$ are equal; rather

$$(\psi, h\eta) - (\psi, h\eta) = \int_0^\infty (\psi''\eta - \psi\eta'')\, dr$$
$$= \alpha(\psi)\beta(\eta) - \beta(\psi)\alpha(\eta) \tag{136b}$$

since the boundary term at infinity does not vanish. Take $\eta = \varphi$, the solution of $h\varphi = 0$ and suppose that ψ is such that $\alpha(\psi) = 1$. Then $(\psi, h\eta) = 0$ so we have that

$$\begin{aligned} a &= \beta(\psi) - (h\psi, \varphi) \\ &= \beta(\psi) - (h\psi, \psi) + (h\psi, (\psi - \varphi)) \\ &= \beta(\psi) - (h\psi, \psi) + (h(\psi - \varphi), (\psi - \varphi)) \end{aligned}$$

The equation

$$a = \beta(\psi) - (h\psi, \psi) + (h(\psi - \varphi), (\psi - \varphi)) \tag{136c}$$

is called the **Kohn variational principle**. Under some circumstances, it can be used to get a rigorous bound on the scattering length:

Theorem XI.61.5 (Rosenberg–Spruch bound) Suppose that $V \in C_0^\infty$ is central and that $-\Delta + V$ has no negative eigenvalues. Let ψ be any function in Q with $\alpha(\psi) = 1$. Then the scattering length a obeys

$$a \geq \beta(\psi) - (h\psi, \psi) \tag{136d}$$

Proof By the Kohn principle, (136c), it suffices that we show $(h\eta, \eta) \geq 0$ for $\eta \in Q$ with $\alpha(\eta) = 0$. Let g be C^∞ on $[0, \infty)$ with $g = 1$ (respectively, $g = 0$) for $r < 1$ (respectively, $r > 2$) and let $g_R(x) = g(x/R)$. Then ηg_R is in L^2 so $0 \leq (g_R\eta, h(g_R\eta))$ by the hypothesis that there are no negative eigenvalues. But $(g_R\eta, h(g_R\eta)) = X + Y + Z$ where

$$X = (g_R^2\eta, h\eta) \to (\eta, h\eta) \qquad \text{as} \quad R \to \infty$$
$$Y = -(g_R\eta, \eta g_R'') \to 0 \qquad \text{as} \quad R \to \infty$$
$$Z = -2(g_R\eta, (\nabla\eta)\nabla g_R) \to 0 \qquad \text{as} \quad R \to \infty$$

where the convergence results follow from $h\eta \leq d_1(1 + r)^{-2}$, $\eta \leq d_2$, $\nabla\eta \leq d_3(1 + r)^{-2}$, $\|g_R''\|_\infty \leq d_4 R^{-2}$, and $\|g_R'\|_\infty \leq d_5 R^{-1}$. Thus $(\eta, h\eta) \geq 0$. ∎

Note that whether (136d) yields an upper or a lower bound on a^2 depends on whether we know that a is positive or negative. For example, by Corollary 3 to Theorem XI.54 and Theorem XI.55, we see that if V is everywhere positive, then (136d) provides an upper bound on a^2.

Appendix 1 to XI.8: Legendre polynomials and spherical Bessel functions

Scattering theory requires some information about certain classes of special functions. The basic properties of Legendre polynomials are most easily derived by defining them in terms of a generating function:

Definition For each $z \in \mathbb{C}$, the function

$$F(x, z) = (1 - 2zx + x^2)^{-1/2}$$

is analytic near $x = 0$. The **Legendre polynomials** $P_\ell(z)$ are defined by

$$P_\ell(z) = (\ell!)^{-1}\left(\frac{d}{dx}\right)^\ell F(x, z)\Big|_{x=0}$$

or equivalently by

$$(1 - 2xz + x^2)^{-1/2} = \sum_{\ell=0}^\infty P_\ell(z)x^\ell$$

Theorem XI.62

(a) $P_\ell(z)$ is a polynomial of degree ℓ with real coefficients.
(b) $P_\ell(1) = 1$; $P_\ell(-z) = (-1)^\ell P_\ell(z)$.
(c) Define f on $\mathbb{R}^3$ by $f(\mathbf{x}) = r^\ell P_\ell(\cos\theta)$ where $r = |\mathbf{x}|$ and $\cos\theta = x_3/r$. Then $-\Delta f = 0$.
(d) (Legendre's equation)

$$(1 - z^2)\frac{d^2}{dz^2}P_\ell(z) - 2z\frac{d}{dz}P_\ell(z) + \ell(\ell + 1)P_\ell(z) = 0$$

(e) $$\int_{-1}^1 P_\ell(z)P_m(z)\, dz = \frac{2}{2\ell + 1}\delta_{\ell m}.$$

(f) $\{(\ell + \frac{1}{2})^{1/2}P_\ell(z)\}_{\ell=0}^\infty$ are an orthonormal basis for $L^2((-1, 1), dz)$.

Proof (a) By the binomial theorem,

$$(1 - 2xz + x^2)^{-1/2} = \sum_{m=0}^{\infty} \binom{-\frac{1}{2}}{m} (-2xz + x^2)^m$$

for x small, where $\binom{k}{m} = k(k-1)\cdots(k-m+1)/m!$ For fixed ℓ, only the terms with $m \le \ell$ can contribute to $(d/dx)^\ell f(x, z)|_{x=0}$. By using the binomial theorem on $(-2xz + x^2)^m$, we see that $\sum_{m=0}^{\ell} \binom{-\frac{1}{2}}{m}(-2xz + x^2)^m$ is a polynomial of two variables of degree ℓ in z. Furthermore, $P_\ell(z) = (-2z)^\ell \binom{-\frac{1}{2}}{\ell} + O(z^{\ell-2})$ so that P_ℓ has degree precisely ℓ.

(b) Since $(1 - 2x + x^2)^{-1/2} = (1-x)^{-1} = \sum_{n=0}^{\infty} x^n$, we see that $P_\ell(1) = 1$. From $f(-x, -z) = f(x, z)$ we obtain $P_\ell(-z) = (-1)^\ell P_\ell(z)$.

(c) Fix $R > 0$. In the region $\{\langle \mathbf{r}, \mathbf{r}' \rangle \in \mathbb{R}^6 \mid r < R < r'\}$ define $g(\mathbf{r}, \mathbf{r}') = |\mathbf{r} - \mathbf{r}'|^{-1}$. Then, for fixed r', $-\Delta g = 0$ in the region $\{\mathbf{r} \mid r < R\}$. Let $\mathbf{r}' = \langle 0, 0, \alpha \rangle$ and $x = r/\alpha$. Then

$$\begin{aligned} |\mathbf{r} - \mathbf{r}'|^{-1} &= (r^2 + r'^2 - 2rr' \cos\theta)^{-1/2} \\ &= (r')^{-1}(1 + x^2 - 2x\cos\theta)^{-1/2} \\ &= (r')^{-1} \sum_{\ell=0}^{\infty} P_\ell(\cos\theta) x^\ell = \sum_{\ell=0}^{\infty} (r')^{-\ell-1} r^\ell P_\ell(\cos\theta) \end{aligned}$$

where we have used the fact that for $z \in (-1, 1)$, $f(x, z)$ has radius of convergence 1 in x. Thus $r^\ell P_\ell(\cos\theta)$ is given inductively by

$$r^\ell P_\ell(\cos\theta) = \lim_{r' \to \infty} (r')^{\ell+1} \left[g(\mathbf{r}, \mathbf{r}') - (r')^{-1} \sum_{k=0}^{\ell-1} P_k(\cos\theta) \left(\frac{r}{r'}\right)^k \right]$$

where the convergence is uniform in $\{\mathbf{r} \mid r < R\}$. By induction in ℓ using the fact that a uniform limit of harmonic functions is harmonic (Problem 89), we conclude that $r^\ell P_\ell(\cos\theta)$ is harmonic.

(d) Since

$$\Delta = r^{-2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + (r^2 \sin\theta)^{-1} \frac{\partial}{\partial\theta} (\sin\theta) \frac{\partial}{\partial\theta} + (r^2 \sin^2\theta)^{-1} \frac{\partial^2}{\partial\varphi^2}$$

(d) follows from (c).

(e) Legendre's equation may be written

$$\frac{d}{dz}(1 - z^2) \frac{d}{dz} P_\ell(z) = -\ell(\ell+1) P_\ell(z)$$

Thus, if $\ell \neq m$, $\int_{-1}^{1} P_\ell(z) P_m(z)\, dz = 0$ since $(d/dz)(1 - z^2)(d/dz)$ is symmetric.

Now, for small x, we compute that on the one hand

$$\begin{aligned} \int_{-1}^{1} \left(\sum_{\ell=0}^{\infty} P_\ell(z) x^\ell \right)^2 dz &= \int_{-1}^{1} (1 - 2xz + x^2)^{-1}\, dz \\ &= x^{-1}[\ln(1+x) - \ln(1-x)] = \sum_{\ell=0}^{\infty} \frac{2}{2\ell+1} x^{2\ell} \end{aligned}$$

while on the other hand, using the fact that for x small and $z \in (-1, 1)$ the convergence of $f(x, z)$ is uniform in z.

$$\int_{-1}^{1} \left(\sum_{\ell=0}^{\infty} x^\ell P_\ell(z) \right)^2 dz = \sum_{\ell=0}^{\infty} \left(\int_{-1}^{1} P_\ell(z)^2\, dz \right) x^{2\ell}$$

on account of the orthogonality relation.

(f) By the Stone–Weierstrass theorem, $\{z^\ell\}_{\ell=0}^{\infty}$ is a total set in $C(-1, 1)$ and so in $L^2(-1, 1)$. Thus, the set arrived at by applying the Gram–Schmidt procedure to $\{z^\ell\}_{\ell=0}^{\infty}$ is an orthonormal basis. But this basis is just $(-1)^\ell(\ell + \frac{1}{2})^{-1/2} P_\ell(z)$. ∎

It is a basic fact about power series that the interior of their region of convergence is always a circle. This follows from the fact that $(z' - z)^{-1} = \sum_{n=0}^{\infty} z^n/(z')^{n+1}$ converges in the region $|z| < |z'|$, that is, if z and z' can be separated by a circle with center at the origin. We want to find the natural regions of convergence for Legendre series, that is, series of the form $\sum_{\ell=0}^{\infty} (2\ell+1) a_\ell P_\ell(z)$. The functions that occur in the Legendre expansion for $(z' - z)^{-1}$ clearly play a critical role. We therefore define:

Definition The **associated Legendre functions** are defined in $\mathbb{C}\backslash[-1, 1]$ by

$$Q_\ell(z) = \frac{1}{2} \int_{-1}^{1} \frac{P_\ell(z')}{z - z'}\, dz'$$

The regions of convergence for Legendre series will be the interiors of certain curves:

Definition Let $z \in \mathbb{C}\backslash[-1, 1]$. By the **canonical ellipse through** z, we mean the unique ellipse passing through z with foci ± 1.

Theorem XI.63

(a) Let z and z' be given so that the canonical ellipse through z lies within the canonical ellipse through z'. Then

$$\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(z)Q_\ell(z') = (z'-z)^{-1} \tag{137}$$

The convergence of (137) is uniform as z and z' run respectively through compact sets C and D so long as there is a canonical ellipse E with C inside E and D outside E.

(b) If f is a function analytic in the interior of a canonical ellipse E, then the series

$$f(z) = \sum_{\ell=0}^{\infty}(2\ell+1)a_\ell P_\ell(z)$$

with

$$a_\ell = \frac{1}{2}\int_{-1}^{1} f(z)P_\ell(z)\,dz \tag{138}$$

converges uniformly on compact subsets of E.

(c) If a_ℓ is any sequence and the series $\sum_{\ell=0}^{\infty}(2\ell+1)a_\ell P_\ell(z)$ converges (respectively, diverges) for some $z_0 \in \mathbb{C}\backslash[-1, 1]$, then it converges absolutely for all z within the canonical ellipse through z_0 (respectively, diverges absolutely for all z outside the ellipse).

Proof (a) We first prove that the series (137) converges uniformly and then establish that the limit is indeed $(z'-z)^{-1}$. Consider the many to one map of $\mathbb{C} \to \mathbb{C}$ given by $\theta \mapsto z = \cos\theta$. The curves $\operatorname{Im}\theta = c$ go into canonical ellipses (Problem 90a); and given z fixed, $|\operatorname{Im}\theta|$ is independent of which $\theta = \cos^{-1} z$ is taken. Since $F(x, z)$ for z fixed has singularities at

$$x = z \pm \sqrt{z^2-1} = \cos\theta \pm i\sin\theta = e^{\pm i\theta}$$

we see that for z fixed, $F(x, z)$ has a radius of convergence $e^{-|\operatorname{Im}\theta|}$. By a Cauchy estimate, for any fixed $H > 1$ and any compact C within the canonical ellipse $|\operatorname{Im}\theta| = \ln H$, $P_\ell(z)H^{-\ell}$ is uniformly bounded as z runs through C and ℓ through 0, 1, ... A similar estimate for $Q_\ell(z)$ (Problem 90b, c, d) shows that for any $H > 1$ and D compact outside the canonical ellipse $|\operatorname{Im}\theta| = \ln H$, $Q_\ell(z)H^\ell$ is uniformly bounded as z runs through D. Given C, D, E as in the hypotheses, find ellipses E' (respectively, E'') given by $|\operatorname{Im}\theta| = \ln H'$ (respectively, $|\operatorname{Im}\theta| = \ln H''$) so that E' (respectively, E'') lies inside (respectively, outside) E and C (respectively, D) lies inside E' (respectively, outside E''). Using the fact that $H'' > H'$, we see that for $z \in C$, $z' \in D$,

$$|P_\ell(z)Q_\ell(z')| \le C[H'/H'']^\ell$$

so the series (137) converges.

If we fix E and z' outside E, then the limiting function $G(z, z')$ is analytic in z for z in E. Moreover,

$$\int_{-1}^{1} P_\ell(z)[G(z, z') - (z'-z)^{-1}]\,dz = 0$$

since $P_\ell(z)(\ell+\frac{1}{2})^{-1/2}$ is an orthonormal basis for $L^2[-1, 1]$. Thus $G(z, z') = (z'-z)^{-1}$ for $z \in (-1, 1)$ and so in all of E by analytic continuation.

(b) Given a compact C inside E, find another canonical ellipse E' so that C is inside E' and E' lies inside E. Then for $z \in C$, we have by the Cauchy theorem

$$f(z) = (2\pi i)^{-1}\oint_{E'}\frac{f(z')}{z'-z}\,dz' = \sum_{\ell=1}^{\infty}P_\ell(z)a_\ell(2\ell+1)$$

where

$$a_\ell = \frac{1}{2\pi i}\oint_{E'} f(z')Q_\ell(z')\,dz'$$

and we have used the uniform convergence proven in (a). Since $P_\ell(z)$ is an orthogonal basis for $L^2(-1, 1)$, (138) holds.

(c) is left to the reader (Problem 91). ∎

Definition The **spherical Bessel functions** $j_\ell(x)$, $x \in \mathbb{C}$, are defined by

$$j_\ell(x) = \frac{e^{-i\pi\ell/2}}{2}\int_{-1}^{1} P_\ell(y)e^{ixy}\,dy$$

Theorem XI.64

(a) $j_\ell(x)$ is real for x real and $j_\ell(-x) = (-1)^\ell j_\ell(x)$.

(b) Each $j_\ell(x)$ is a finite linear combination of terms of the form $x^{-m}\cos x$ and $x^{-m}\sin x$ with $m \le \ell + 1$.

(c) $j_\ell(x)$ is an entire function of x with $j_\ell(x) = O(x^\ell)$ for $x \to 0$.

(d) (Bessel's equation)

$$-\frac{d^2}{dx^2}[xj_\ell(x)] + \frac{\ell(\ell+1)}{x^2}[xj_\ell(x)] = [xj_\ell(x)]$$

(e) $[xj_\ell(x) - \sin(x - \frac{1}{2}\pi\ell)] = O(x^{-1})$ as $x \to \infty$.

(f) If $\mathbf{e}$ is the unit vector $\langle 0, 0, 1\rangle$ and $\mathbf{r} \cdot \mathbf{e} = r\cos\theta$, then

$$e^{ik\mathbf{e}\cdot\mathbf{r}} = \sum_{\ell=0}^{\infty} e^{i\pi\ell/2}(2\ell + 1)j_\ell(kr)P_\ell(\cos\theta)$$

where the series converges uniformly as k and $\mathbf{r}$ run through compact sets of $\mathbb{R}$ and $\mathbb{R}^3$ respectively.

Proof (a) $\overline{j_\ell(x)} = \frac{1}{2}e^{i\pi\ell}e^{-i\pi\ell/2}\int_{-1}^{1} P_\ell(y)e^{-ixy}\,dy$. Changing y into $-y$ and using $P_\ell(-y)e^{i\pi\ell} = P_\ell(y)$, we conclude that j_ℓ is real. Since P_ℓ is real,

$$j_\ell(-x)e^{+i\pi\ell/2} = \overline{j_\ell(x)e^{i\pi\ell/2}} = j_\ell(x)e^{-i\pi\ell/2}$$

or $j_\ell(-x) = (-1)^\ell j_\ell(x)$.

(b) Using $y^n e^{ixy} = (i^{-1}\,d/dx)^n e^{ixy}$, we see that

$$j_\ell(x) = e^{-i\pi\ell/2}P_\ell\left(\frac{1}{i}\frac{d}{dx}\right)\left[\frac{\sin x}{x}\right]$$

By induction, $(d/dx)^m x^{-1}\sin x$ is a finite linear combination of terms of the form $x^{-k}\sin x$ and $x^{-k}\cos x$ with $k \le m + 1$ so (b) follows.

(c) j_ℓ is the Fourier transform of a distribution of compact support and therefore an entire function of x. Moreover

$$\left.\frac{d^k j_\ell}{dx^k}\right|_{x=0} = \frac{1}{2}e^{-i\pi\ell/2}(i)^k\int_{-1}^{1} y^k P_\ell(y)\,dy$$

is zero if $k < \ell$ by the orthogonality relations for the Legendre polynomials. Thus $j_\ell(x) = O(x^\ell)$ as $x \to 0$.

(d) Let χ be the characteristic function of $(-1, 1)$ and let F be the distribution χP_ℓ. Then

$$\frac{dF}{dy} = \chi\frac{dP_\ell}{dy} + P_\ell(1)\,\delta(y - 1) - P_\ell(-1)\,\delta(y + 1)$$

so

$$(1 - y^2)\frac{dF}{dy} = \chi(1 - y^2)\frac{dP_\ell}{dy}$$

and thus

$$\frac{d}{dy}(1 - y^2)\frac{dF}{dy} = \chi\frac{d}{dy}(1 - y^2)\frac{dP_\ell}{dy}$$
$$= -\ell(\ell + 1)F$$

by (d) of Theorem XI.62. Taking Fourier transforms,

$$x\left(1 + \frac{d^2}{dx^2}\right)xj_\ell(x) = \ell(\ell + 1)j_\ell(x)$$

which proves Bessel's equation.

(e) Since $e^{ixy} = (ix)^{-1}(d/dy)e^{ixy}$, integration by parts yields

$$j_\ell(x) = \frac{e^{-i\pi\ell/2}}{2}\frac{1}{ix}[e^{ix}P_\ell(1) - e^{-ix}P_\ell(-1)] - \frac{e^{-i\pi\ell/2}}{2ix}\int_{-1}^{1} e^{ixy}\frac{d}{dy}P_\ell(y)\,dy$$

By another integration by parts, one can see that the second term is $O(x^{-2})$ at infinity. Using $P_\ell(1) = 1$, $P_\ell(-1) = (-1)^\ell$, the first term can be rewritten as $x^{-1}\sin(x - \frac{1}{2}\pi\ell)$.

(f) For k and r fixed, the function

$$f(r, k, \eta) = e^{ikr\eta}$$

is an entire function of η with uniform bounds as k, r, and η run through compact subsets of $\mathbb{R}$ (respectively, $\mathbb{C}$). Thus the Legendre series

$$f(r, k, \eta) = \sum_{\ell=0}^{\infty}(2\ell + 1)a_\ell(k, r)P_\ell(\eta)$$

converges uniformly on such compact sets. Since

$$a_\ell(k, r) = \frac{1}{2}\int_{-1}^{1} P_\ell(\eta)f(r, k, \eta)\,d\eta$$

we see that $a_\ell(r) = e^{i\pi\ell/2}j_\ell(kr)$ by the definition of $j_\ell(x)$. ∎

Appendix 2 to XI.8: Jost solutions for oscillatory potentials

In this appendix and the next we shall consider certain classes of potentials with severe oscillations at infinity. To some extent, these examples are mathematical curiosities—but they are of theoretical interest for several reasons: First, these examples illuminate the modifications of the wave operators considered in Section 9; and secondly, there are connections with the phenomenon of positive eigenvalues (see Section XIII.13).

The net effort of these two appendices will be to show that so long as the average of V falls off, it does not matter that V fails to fall off. One can understand this heuristically in terms of the spreading of smooth free wave packets. Consider the following examples:

Example 1 Let

$$V(r) = (1 + r^2)^{-1} e^r \sin(e^r) \tag{139}$$

V is clearly very singular at infinity. But its average is not since an integration by parts shows that

$$\int_r^R V(x)\,dx$$

$$= (1 + r^2)^{-1} \cos(e^r) - (1 + R^2)^{-1} \cos(e^R) + 2\int_r^R x(1 + x^2)^{-2} \cos(e^x)\,dx$$

so that

$$W(r) = -\lim_{R\to\infty} \int_r^R V(x)\,dx \tag{140}$$

exists and is "short-range" in the sense that

$$|W(r)| \leq C(1 + r^2)^{-1}$$

Because of this falloff of the average of V, it turns out that $-\Delta + V$ can be defined as a sum of forms and that it is bounded from below in spite of the fact that V is so unbounded. For $V(r) = \partial W/\partial r$ and thus on $\mathbb{R}^n$

$$V(x) = \sum_{i=1}^n \frac{\partial}{\partial x_i} G_i(\mathbf{x}) + K(x)$$

where $G_i(\mathbf{x}) = x^{-1} x_i W(x)$ and $K(x) = -(n-1)x^{-1}W(x)$. On the basis of this we claim that for any ε, there is a C_ε with

$$(\varphi, V\varphi) \leq \varepsilon(\varphi, (-\Delta)\varphi) + C_\varepsilon(\varphi, \varphi) \tag{141}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^n)$. K is $-\Delta$-form bounded with relative bound zero. Moreover, by an integration by parts followed by the Schwarz inequality,

$$|(\varphi, (\partial G_i/\partial x_i)\varphi)| = \left|\int \frac{\partial G_i}{\partial x_i} |\varphi|^2\,dx\right| = 2|\mathrm{Re}(\varphi, G_i\,\partial\varphi/\partial x_i)|$$

$$\leq (\varphi, G_i^2\varphi)^{1/2}(\partial\varphi/\partial x_i, \partial\varphi/\partial x_i)^{1/2}$$

so that (141) follows since G_i^2 is $-\Delta$-form bounded with relative bound zero. From (141), $(\varphi, V\varphi)$ can be extended to $Q(-\Delta)$ and $-\Delta + V$ is a semibounded closed quadratic form on $Q(-\Delta)$. We warn the reader that for arbitrary $\varphi \in Q(-\Delta)$, it may *not* be true that $\int |V(x)|\,|\varphi(x)|^2\,dx < \infty$; $(\varphi, V\varphi)$ is defined via a limiting argument. One can actually develop a scattering theory for $-\Delta + V$ by mimicking the ideas in Theorem XI.31 (see Problem 92) or the methods of Section XIII.8 (see the reference in the Notes). Here we want to consider Jost functions for such V's.

Example 2 Let

$$V(r) = \sum_{j=1}^m \gamma_j r^{-1} \sin(\alpha_j r) + Q(r) \tag{142a}$$

with

$$|Q(r)| \leq C(1 + r^2)^{-\frac{1}{2}-\varepsilon} \tag{142b}$$

for some $\varepsilon > 0$ and C. In this case V is bounded, so there is no problem defining $-\Delta + V$. Two subtle phenomena are associated with $-\Delta + V$. In the first place, there is a potential of the form (142) so that $(-\Delta + V)\varphi = \varphi$ has a square integrable solution even though $V \to 0$ at infinity. (See Example 1 of Section XIII.13 and the discussion there.) In the second place, $V(r)$ does not fit into the framework of potentials whose scattering theory we have developed since $\int_1^\infty |V(r)|\,dr = \infty$. In Section 9 we shall develop a modified scattering theory for potentials like the Coulomb potential. Unfortunately, the estimates needed to make the Coulomb theory work are not applicable to potentials of the form of (142). However, that theory suggests the type of scattering theory one might expect for potentials of this form. In Section 9 we make a modification of the free dynamics in defining time-dependent wave operators. As $t \to \infty$, this modification diverges in the Coulomb case, and so without it the wave operators do not exist. Because the indefinite integral (140) exists if V obeys (142), the modification of Section 9 actually converges in this case; so if the modified wave operators exist, so do the original wave operators. This suggests that the ordinary wave operators exist for this case. By investigating Jost solutions for these potentials we shall see when positive eigenvalues exist and also develop the scattering theory. This scattering theory appears in the next appendix.

Since we are here interested in the problems associated with oscillations at infinity, we shall suppose throughout this appendix that $V(r)$ is continuous and locally bounded. Our methods can be easily modified to accommodate local singularities in V. In understanding Examples 1 and 2, the following result is needed; it and its corollaries are easily extended to the case where X is a Banach space. In our applications, dim $X = 2$.

Proposition Let X be a finite-dimensional normed vector space. Let $C(x)$ be a continuous function on $[R_0, \infty)$ with values in $\mathscr{L}(X)$. Let $D(x, y)$

be a measurable function on $Q \equiv \{\langle x, y\rangle | R_0 \le x \le y < \infty\}$ with values in $\mathscr{L}(X)$.

(a) Suppose that

$$\gamma \equiv \sup_{x \ge R_0} \|C(x)\| + \sup_{x \ge R_0} \int_x^\infty \|D(x, y)\|\, dy < 1$$

Then, for any $u_0 \in X$, the equation

$$u(x) = u_0 + C(x)u(x) + \int_x^\infty D(x, y)u(y)\, dy \tag{143}$$

has a unique solution in $L^\infty(R_0, \infty)$. Furthermore, this solution is continuous.

(b) Moreover, if

$$\gamma(r) \equiv \sup_{x \ge r} \|C(x)\| + \sup_{x \ge r} \int_x^\infty \|D(x, y)\|\, dy$$

goes to zero as $r \to \infty$, then $\lim_{x\to\infty} u(x) = u_0$ and for $x > R_0$,

$$\|u(x) - u_0\| \le \gamma(x)[1 - \gamma(x)]^{-1}\|u_0\|$$

(c) Suppose that C is continuously differentiable, that D is continuous on Q, and that for each fixed x,

$$f_\varepsilon(y) = \varepsilon^{-1}[D(x + \varepsilon, y) - D(x, y)]$$

converges in $L^1(\mathbb{R}, \infty)$ to a function, denoted by $\partial D/\partial x$, which is continuous in x in L^1 sense. Then the solution u of (143) is continuously differentiable and

$$u'(x) = C'(x)u(x) + C(x)u'(x) - D(x, x)u(x) + \int_x^\infty \frac{\partial D}{\partial x}(x, y)u(y)\, dy \tag{144}$$

(a) and (b) remain true if the constant u_0 is replaced by a continuous function $u_0(x)$ with $\sup_{x\ge R_0} \|u_0(x)\| = Q_0 < \infty$ so long as $\|u_0\|$ is replaced by Q_0 in all estimates. (c) still holds in this case so long as $u_0(x)$ is C^1 and a term $u_0'(x)$ is added on the right side of (144).

Proof (a) Define $u_n(x)$ inductively by $u_0(x) = u_0$ and

$$u_n(x) = C(x)u_{n-1}(x) + \int_x^\infty D(x, y)u_{n-1}(y)\, dy$$

One easily proves inductively that $u_n(x)$ is continuous and

$$\sup_{|x|\ge r} \|u_n(x)\| \le \gamma(r)^n\|u_0\| \tag{145}$$

Since $\gamma(R_0) = \gamma < 1$, $\sum_{n=0}^N u_n(x)$ converges uniformly to a continuous function $u(x)$ that obeys (143). If v is any solution of (143) in $L^\infty(R_0, \infty)$, by iterating (143), one finds that

$$\left\| v - \sum_{n=0}^N u_n(x) \right\| \le \gamma^{N+1}\|v\|_\infty$$

so taking $N \to \infty$, $v = u$.

(b) By (145),

$$\|u - u_0\| \le \sum_{n=1}^\infty \gamma(r)^n\|u_0\| = \gamma(r)(1 - \gamma(r))^{-1}\|u_0\|$$

(c) Under the hypothesis, u_n is inductively seen to be continuously differentiable with

$$u_n'(x) = C'(x)u_{n-1}(x) + C(x)u_{n-1}'(x) - D(x, x)u_{n-1}(x) + \int_x^\infty \frac{\partial D}{\partial x}(x, y)u_{n-1}(y)\, dy$$

Using (145), one can prove (Problem 93) the following bounds inductively:

$$|u_n'(x)| \le n\gamma^n\|u_0\|A(x), \qquad x \ge R_0$$

where

$$A(x) = \gamma^{-1}\left(\|C'(x)\| + \|D(x, x)\| + \int_x^\infty \left\|\frac{\partial D}{\partial x}(x, y)\right\| dy\right)$$

It follows that $\sum_{n=0}^\infty u_n'(x)$ converges uniformly on any compact subset of $[R_0, \infty)$, so that $u(x)$ is differentiable with derivative $\sum_{n=0}^\infty u_n'(x)$. Thus (144) holds. The case when u_0 is x-dependent is left to the reader (Problem 93). ∎

Theorem XI.65 Let $A(x)$ be a continuous function from $[R_0, \infty)$ to $\mathscr{L}(X)$, the bounded operators on a finite-dimensional normed linear space. Assume that $\|A(x)\| \in L^1(R, \infty)$. Suppose that $u_0 \in X$. Then there exists a unique continuously differentiable function $u(x, u_0)$ so that

$$\frac{du}{dx} = A(x)u(x)$$

and $\lim_{x\to\infty} u(x) = u_0$. Every nonzero solution has a nonzero limit as $x \to \infty$. Moreover, $\|u(x) - u_0\| \le 2\|u_0\| \int_x^\infty \|A(y)\|\, dy$ for all x with $\int_x^\infty \|A(y)\|\, dy < \frac{1}{2}$.

Proof Pick R_1 so that $\int_{R_1}^{\infty} \|A(x)\|\, dx < 1$. Then, by the proposition,

$$u(x) = u_0 - \int_x^{\infty} A(y)u(y)\, dy$$

has a unique solution on $[R_1, \infty)$ that is continuously differentiable with $u'(x) = A(x)u(x)$. Using local existence and uniqueness, this can be continued to $[R, \infty)$. Picking a basis for X, we can find n linearly independent solutions with different linearly independent limits at infinity. By local uniqueness, these span all solutions yielding uniqueness together with the fact that every solution has a limit. The last bound follows from (b) of the proposition. ∎

Example 3 Consider the equation

$$-\varphi''(x) + V(x)\varphi(x) = k^2\varphi(x)$$

on $[1, \infty)$ where $\int_1^{\infty} |V(x)|\, dx < \infty$. Let $\Psi(x) = \binom{\varphi(x)}{\varphi'(x)}$. Then $\Psi'(x) = C(x)\Psi(x)$ where

$$C(x) = \begin{pmatrix} 0 & 1 \\ V(x) - k^2 & 0 \end{pmatrix}$$

Let $\varphi_{\pm}$ be the vector valued functions

$$\varphi_{\pm}(x) = \begin{pmatrix} e^{\pm ikx} \\ \pm ike^{\pm ikx} \end{pmatrix}$$

and write $\Psi(x) = \alpha(x)\varphi_+(x) + \beta(x)\varphi_-(x)$ where α and β are complex-valued functions. Then $q = \binom{\alpha}{\beta}$ obeys $q(x) = M(x)\Psi(x)$ with

$$M(x) = (2ik)^{-1}\begin{pmatrix} ike^{-ikx} & e^{-ikx} \\ ike^{ikx} & -e^{ikx} \end{pmatrix}$$

Thus

$$q'(x) = D(x)q(x) \tag{146a}$$

where $D(x) = M'(x)M(x)^{-1} + M(x)C(x)M(x)^{-1}$ so

$$D(x) = (2ik)^{-1}V(x)\begin{pmatrix} 1 & e^{-2ikx} \\ -e^{2ikx} & -1 \end{pmatrix} \tag{146b}$$

Applying Theorem XI.65 to (146), we see that if $\int_1^{\infty} |V(x)|\, dx < \infty$, then (146) has solutions asymptotic to any q_0 as $x \to \infty$. Taking $q = \binom{1}{0}$, we find a solution φ of the Schrödinger equation with $|\varphi(x) - e^{ikx}| + |\varphi'(x) - ike^{ikx}| \to 0$ as $x \to \infty$. We thus have a proof of the existence of Jost solutions somewhat independent of the one given in the section.

Example 4 Consider solutions of $-f''(r) + \ell(\ell+1)r^{-2}f(r) = k^2 f(r)$. Proceeding as in the above example, one can show that any real-valued solution obeys $|f(r) - C\sin(kr + D)| = O(r^{-1})$ and in particular

$$|krj_\ell(kr) - \sin(kr - \tfrac{1}{2}\pi\ell)| = O(r^{-1})$$

To handle Example 2, we need an interesting extension of Theorem XI.65.

Theorem XI.66 (Dollard–Friedman theorem) Let $A(x)$ be a continuous function from $[R, \infty)$ to $\mathscr{L}(X)$, the bounded operators on a finite-dimensional normed linear space. Suppose that $A = A_1 + A_2$ where

(i) $\|A_1(\cdot)\| \in L^1(R, \infty)$.
(ii) $B(x) = -\lim_{r\to\infty} \int_x^r A_2(y)\, dy$ exists.
(iii) $\|B(\cdot)A(\cdot)\| \in L^1(R, \infty)$.

Then there exists a unique continuously differentiable X-valued function $u(x; u_0)$ such that

$$\frac{du}{dx} = A(x)u(x)$$

and $\lim_{x\to\infty} u(x; u_0) = u_0$. Every nonzero solution of the differential equation has a nonzero limit as $x \to \infty$ and

$$|u(x; u_0) - u_0| \leq 2\left(\sup_{y\geq x} \|B(y)\| + \int_x^{\infty} \|A_1(y)\|\, dy + \int_x^{\infty} \|B(y)A(y)\|\, dy\right)\|u_0\| \tag{147}$$

for all x such that the expression in ( ) is smaller than $\frac{1}{2}$.

Proof We begin with some manipulation of the formal equation

$$u(x) = u_0 - \int_x^{\infty} A(y)u(y)\, dy$$

Write $A_2(y) = dB(y)/dy$ and integrate by parts. The boundary term at infinity should vanish since

$$\lim_{y\to\infty} \|B(y)\| = 0 \tag{148}$$

on account of the convergence of the integral defining $B(y)$. Using $u'(y) = A(y)u(y)$, we find that

$$u(x) = u_0 + B(x)u(x) - \int_x^\infty [A_1(y) - B(y)A(y)]u(y)\,dy \tag{149}$$

Having arrived at (149) formally, we solve it and then show that the solution has the required properties.

Let

$$\gamma(x) = \sup_{y \geq x} \|B(y)\| + \int_x^\infty (\|A_1(y)\| + \|B(y)A(y)\|)\,dy$$

By (148) and the hypotheses, $\gamma(x) \to 0$ as $x \to \infty$; so, by the proposition, (149) has solutions in $[R_1, \infty)$ for R_1 sufficiently large and the solutions obey (147). By (c) of the proposition, the solution is C^1 and

$$u'(x) = B(x)u'(x) + A_2(x)u(x) + [A_1(x) - B(x)A(x)]u(x)$$

so that

$$(1 - B(x))u'(x) = (1 - B(x))A(x)u(x)$$

By (148), $1 - B(x)$ is invertible for x large; thus, we have the desired solution of the differential equation for x large. The rest of the proof follows by local solvability as in Theorem XI.65. ∎

Example 2, revisited We seek solutions of $-\varphi''(x) + V(x)\varphi(x) = k^2\varphi(x)$ where $V(x)$ has the form of (142). As in Example 3, we begin by writing the equation in the form of (146). Write $D = D_1 + D_2$ where D_1 comes from the $Q(x)$ term and D_2 from the $r^{-1}\sin(\alpha_j r)$ terms. D_1 is clearly in L^1. Moreover, since

$$\int_r^x y^{-1}e^{i\beta y}\,dr = (i\beta y)^{-1}e^{i\beta y}\Big]_r^x + (i\beta)^{-1}\int_r^x y^{-2}e^{i\beta y}\,dy$$

we see that for $\beta \neq 0$, $\lim_{x\to\infty} \int_r^x y^{-1}e^{i\beta y}\,dy$ exists and the resulting function is bounded by r^{-1}. It follows that, so long as $\alpha_j \neq \pm 2k$ for all j, $B(r) = \int_r^\infty D_2(x)\,dx$ exists as an improper integral, and $BD \in L^1$ with $\int_r^\infty \|B(y)D(y)\|\,dy = O(r^{-1})$. As a result, Theorem XI.66 is applicable and immediately yields a proof of (a) and (b) of the following theorem.

Theorem XI.67 Let V have the form of (142).

(a) Let k be a real number with $k \neq 0, \pm\frac{1}{2}\alpha_1, \ldots, \pm\frac{1}{2}\alpha_m$. Then every nonzero solution of $-\varphi'' + V\varphi = k^2\varphi$ satisfies

$$\lim_{x\to\infty} [\varphi(x) - ae^{ikx} - be^{-ikx}] = 0$$

for suitable a and b. In particular, $-\varphi'' + V\varphi = k^2\varphi$ has no nonzero square integrable solutions.

(b) For any k as in (a), there exists a unique solution $\varphi(x; k)$ of $-\varphi'' + V\varphi = k^2\varphi$ on $[1, \infty)$ satisfying

$$|\varphi(x; k) - e^{-ikx}| \leq c_k |x|^{-\alpha}, \qquad x \geq 1$$

with $\alpha = \min\{1, 2\varepsilon\}$ where ε is given in (142b). Moreover, c_k can be chosen independently of k as k runs through a compact subset of $\{k \in \mathbb{R} \mid k \neq 0, \pm\frac{1}{2}\alpha_1, \ldots, \pm\frac{1}{2}\alpha_m\}$.

(c) Suppose that $k = \frac{1}{2}\alpha_j$ for some j. Then there exists a solution u of $-\varphi'' + V\varphi = k^2\varphi$ that satisfies

$$u = \begin{cases} r^{-\gamma_j/2\alpha_j}(\cos(\frac{1}{2}\alpha_j r) + o(1)), & \gamma_j/\alpha_j > 0 \\ r^{+\gamma_j/2\alpha_j}(\sin(\frac{1}{2}\alpha_j r) + o(1)), & \gamma_j/\alpha_j < 0 \end{cases}$$

For a proof of part (c), see the reference in the Notes and Problems 97 and 98. The point of part (c) is that when γ_j is bigger than α_j, there is a solution of the Schrödinger equation that is square integrable at ∞. In general, if one has a one-parameter family of such potentials, one of the solutions will obey the requisite boundary conditions at the origin. Therefore, there exist Schrödinger operators with positive eigenvalues embedded in the continuous spectrum. This is further discussed in Section XIII.13.

In the next appendix we shall see that so long as $\varepsilon > \frac{1}{4}$, part (b) of the theorem can be used to prove that $\Omega^\pm(-\Delta + V, -\Delta)$ exist and have equal ranges.

The proof of the Dollard–Friedman theorem and the solution of the problem posed in Example 2 involved integration by parts in the obvious integral equation. The same method works in Example 1, but the "suitable equation" is not given directly by (146) but rather by the Jost integral equation (126). We remark that one can "derive" the Jost equation easily from (146).

Example 1, revisited We begin with the Jost equation and formally manipulate under the assumption that $V(r) = \partial W/\partial r$ with

$\int_x^\infty |W(r)|\,dr < \infty$. Integrating by parts in

$$\varphi(x) = e^{-ikx} - \int_x^\infty \frac{\sin k(x-y)}{k} V(y)\varphi(y)\,dy$$

and dropping the boundary term at infinity, we obtain

$$\varphi(x) = e^{-ikx} - \int_x^\infty W(y)[\cos(kx-ky)\varphi(y) - k^{-1}\sin(kx-ky)\varphi'(y)]\,dy \tag{150a}$$

and similarly, integrating by parts in

$$\varphi'(x) = -ike^{-ikx} - \int_x^\infty \cos(kx-ky)V(y)\varphi(y)\,dy$$

we obtain

$$\varphi'(x) = -ike^{-ikx} + W(y)\varphi(y) + \int_x^\infty W(y)[k\sin(kx-ky)\varphi(y) + \cos(kx-ky)\varphi'(y)]\,dy \tag{150b}$$

Rewriting (150) as a system of equations for $\langle\varphi, \varphi'\rangle$, we see that it has a C^1 solution on account of the proposition. Using part (c) of the proposition, one easily sees that the resulting solution obeys $\varphi''(x) = V(x)\varphi(x) - k^2\varphi(x)$. We summarize with:

Theorem XI.68 Let $V(r)$ be a continuous function with $V(r) = \partial W/\partial r$ where $W \in L^1[1, \infty)$. Then:

(a) $-\varphi'' + V\varphi = k^2\varphi$ has no nonzero square integrable solution for $k \neq 0$.

(b) Suppose that $|W(x)| \leq C|x|^{-1-\varepsilon}$. Then, for any $k \neq 0$, there is a solution $\varphi(x; k)$ of $-\varphi'' + V\varphi = k^2\varphi$ in $[1, \infty)$ with

$$|\varphi(x, k) - e^{-ikx}| \leq c(k)|x|^{-\varepsilon}, \qquad x \geq 1$$

$c(k)$ can be chosen independently of k for $|k| \geq k_0 > 0$.

Appendix 3 to XI.8: Jost solutions and the fundamental problems of scattering theory

In this appendix we consider cases where one has regular solutions of the Schrödinger equation $u_\ell(x; k)$ and good control on how fast $|u_\ell(x; k) - \sin(kx - \frac{1}{2}\ell\pi + \delta_\ell)|$ goes to zero as $|x|$ goes to ∞. From this information

we shall prove that $\Omega^\pm$ exist, that Ran Ω^+ = Ran Ω^- and that S is multiplication by $e^{2i\delta_\ell(k)}$ in the representation where energy and angular momentum are diagonal. This will enable us to recover some of the results of the section and more importantly to develop scattering theory for some of the potentials of Appendix 2. Moreover, it will shed some light on the invariance principle for wave operators. Throughout, we use the symbol $\hat{x}$ for $\mathbf{x}/|x|$. The basic result is:

Theorem XI.69 Let $V(\mathbf{x})$ be a central potential on $\mathbb{R}^3$ so that $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Suppose that for each $\ell = 0, 1, \ldots$, there is a closed set $\mathscr{E}_\ell$ of measure zero in $(0, \infty)$ such that for each $k \in (0, \infty)\backslash\mathscr{E}_\ell$, there is a real-valued distributional solution

$$\varphi(\mathbf{x}; k) = (k|\mathbf{x}|)^{-1}u_\ell(|\mathbf{x}|; k)Y_{\ell m}(\hat{x})$$

of $(-\Delta + V)\varphi_\ell = k^2\varphi_\ell$ obeying

$$|u_\ell(k, r) - \sin(kr - \tfrac{1}{2}\ell\pi + \delta_\ell(k))| \leq c_\ell(k)(1 + |r|)^{-\frac{1}{2}-\gamma} \tag{151}$$

for a fixed $\gamma > 0$. Suppose that $\varphi_\ell(\mathbf{x}; \cdot)$ and $\delta_\ell(\cdot)$ are measurable and that $\sup_{k\in K} c_\ell(k) < \infty$ for every compact subset K of $(0, \infty)\backslash\mathscr{E}_\ell$. Then, $\Omega^\pm(-\Delta + V, -\Delta)$ exist, Ran Ω^+ = Ran Ω^-, and $S = (\Omega^-)^*\Omega^+$ is given by

$$S\left[\sum_{\ell,m} Y_{\ell m}(\hat{x})\int_0^\infty j_\ell(k|x|)f_{\ell m}(k)\,dk\right] = \sum_{\ell,m} Y_{\ell m}(\hat{x})\int_0^\infty j_\ell(k|x|)e^{2i\delta_\ell(k)}f_{\ell m}(k)\,dk \tag{152}$$

Proof Fix ℓ, m, and $f \in C_0^\infty((0, \infty)\backslash\mathscr{E}_\ell)$. Let

$$\psi(\mathbf{x}) = Y_{\ell m}(\hat{x})\int_0^\infty (kx)^{-1}u_\ell(x; k)f(k)\,dk$$

$$\psi_\pm^{(0)}(\mathbf{x}) = Y_{\ell m}(\hat{x})\int_0^\infty j_\ell(kx)e^{\mp i\delta_\ell(k)}f(k)\,dk$$

Using (151) and $f \in C_0^\infty$, one easily sees that ψ and $\psi_\pm^{(0)}$ are in $L^2(\mathbb{R}^3)$ (Problem 94). We shall show that

$$\lim_{t\to\mp\infty} \|e^{-itH}\psi - e^{-itH_0}\psi_\pm^{(0)}\| = 0 \tag{153}$$

Once (153) is proven, we conclude that $\Omega^\pm$ exist for a dense set and obtain formulas for $\Omega^\pm$ that establish Ran Ω^+ = Ran Ω^- and that (152) holds. Let C be complex conjugation. Then $e^{-itH_0}C = Ce^{itH_0}$ and $e^{-itH}C = Ce^{itH}$, so (153) need only be proven for the case $t \to -\infty$.

Since $-\Delta + V = H$ obeys $H\varphi_\ell(\cdot\,; k) = k^2\varphi_\ell(\cdot\,; k)$ in distributional sense, we see that for $\eta \in C_0^\infty(\mathbb{R}^3)$,

$$(H\eta, \psi) = (\eta, \tilde{\psi})$$

where $\tilde{\psi}$ is given by the formula for ψ except that $f(k)$ is replaced by $k^2 f(k)$. Since H is essentially self-adjoint on C_0^∞, $\psi \in D(H)$ and $H\psi = \tilde{\psi}$. Repeating this and using the fact that $f \in C_0^\infty$, we see that

$$\psi(\mathbf{x}, t) \equiv (e^{-itH}\psi)(\mathbf{x}) = Y_{\ell m}(\hat{x}) \int_0^\infty (kx)^{-1} u_\ell(x; k) e^{-itk^2} f(k)\, dk$$

Similarly,

$$\psi_+^{(0)}(\mathbf{x}, t) \equiv (e^{-itH_0}\psi)(\mathbf{x}) = Y_{\ell m}(\hat{x}) \int_0^\infty j_\ell(kx) e^{-itk^2} e^{-i\delta_\ell(k)} f(k)\, dk$$

Now, *define* $\eta(\mathbf{x}, t)$ by

$$\eta(\mathbf{x}, t) = Y_{\ell m}(\hat{x}) \int_0^\infty (kx)^{-1} \sin(kx - \tfrac{1}{2}\ell\pi + \delta_\ell(k)) e^{-itk^2} f(k)\, dk$$

Then

$$\alpha_t(\mathbf{x}) \equiv |\psi(\mathbf{x}, t) - \eta(\mathbf{x}, t)| = |Y_{\ell m}(\hat{x})| \left| \int_0^\infty (kx)^{-1} q(x, k) e^{-itk^2} f(k)\, dk \right|$$

where $q(x, k) = u(x; k) - \sin(kx - \frac{1}{2}\ell\pi + \delta_\ell(k))$. Now, for each fixed x, $(kx)^{-1}q(x, k)f(k)$ is in $L^1(0, \infty)$ as a function of k by (151), so $\alpha_t(x) \to 0$ as $t \to \pm\infty$ by the Riemann–Lebesgue lemma. Moreover, by (151),

$$|\alpha_t(\mathbf{x})| \leq C |Y_{\ell m}(\hat{x})| x^{-1}(1 + x)^{-\frac{1}{2}-\gamma}$$

for all t. Thus, by the dominated convergence theorem, $\int |\alpha_t(x)|^2\, d^3x \to 0$ as $t \to \pm\infty$. This reduces the proof of (153) to showing that

$$\int |\psi_+^{(0)}(x, t) - \eta(x, t)|^2\, d^3x \to 0 \qquad \text{as} \quad t \to -\infty$$

Let

$$\zeta_\pm(\mathbf{x}, t) = Y_{\ell m}(\hat{x}) \int (kx)^{-1} e^{\pm ikx} e^{\pm i\delta_\ell(k)} e^{\mp i\ell\pi/2} e^{-ik^2t} f(k)\, dk$$

By Lemma 3 of Section 3,

$$\lim_{t \to -\infty} \int |\zeta_+(\mathbf{x}, t)|^2\, d^3x = 0$$

so

$$\lim_{t \to -\infty} \int |\eta(\mathbf{x}, t) - \tfrac{1}{2}i\zeta_-(\mathbf{x}, t)|^2\, d^3x = 0$$

The same set of arguments we have just made leads to

$$\lim_{t \to -\infty} \int |\psi_+^{(0)}(\mathbf{x}, t) - \tfrac{1}{2}i\zeta_-(\mathbf{x}, t)|^2\, d^3x = 0$$

if we use $|krj_\ell(kr) - \sin(kr - \frac{1}{2}\ell\pi)| \leq C(k)(1 + |r|)^{-1}$ in place of (151). We conclude that (153) holds. ∎

In the above, φ was a generalized eigenfunction with eigenvalue $E(k) = k^2$. The exact functional form of $E(k)$ played no role in the proof, which goes through as long as E is strictly monotone. This not only demonstrates that an invariance principle holds in the context of the above theorem, but makes transparent the reason that invariance holds at all.

Corollary 1 If $V(\mathbf{x})$ is a central potential satisfying

$$|V(x)| \leq C(1 + |x|)^{-\frac{1}{2}-\varepsilon}$$

($\varepsilon > 0$), then $\Omega^\pm(-\Delta + V, -\Delta)$ exist, $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^-$, and the S-operator is given by (152).

Of course, this result is not a new one for us—stronger results are proven in Section 8—but the proof is quite direct. The following result is based on Theorem XI.67.

Corollary 2 Let

$$V(x) = \sum_{j=1}^m \gamma_j r^{-1} \sin(\alpha_j r) + Q(r)$$

with $|Q(r)| \leq C(1 + r)^{-\frac{1}{2}-\varepsilon}$. Then $\Omega^\pm(-\Delta + V, -\Delta)$ exist, $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^-$ and the S-operator is given by (152).

By modifying the arguments slightly, one can accommodate some of the highly oscillatory potentials of Theorem XI.68 (Problem 95). Moreover, by appealing to results from the theory of ordinary differential equations, one can prove that $\operatorname{Ran}\Omega^\pm = \operatorname{Ran} P_{\text{ac}}(-\Delta + V)$ and that $-\Delta + V$ has no singular continuous spectrum in the situations described by Corollaries 1 and 2. Finally, we note a version of Theorem XI.69 for noncentral potentials.

Theorem XI.70 Let $V(\mathbf{x})$ be a measurable function on $\mathbb{R}^3$ so that $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Suppose that there is a closed set $\mathscr{E}$ of measure zero in $\mathbb{R}^3$, so that for each $\mathbf{k} \in \mathbb{R}^3\backslash\mathscr{E}$, there is a distributional solution $\varphi(\mathbf{x}, \mathbf{k})$ of $(-\Delta + V)\varphi = k^2\varphi$ obeying

$$|\varphi(\mathbf{x}, \mathbf{k}) - e^{i\mathbf{k}\cdot\mathbf{x}} - \gamma(\mathbf{k}, \hat{x})x^{-1}e^{ikx}| \leq C(\mathbf{k})(1 + x)^{-\frac{1}{2}-\varepsilon} \tag{154}$$

for $|x| \geq 1$. Suppose that φ and γ are measurable functions, that $\overline{\varphi(\mathbf{x}, \mathbf{k})} = \varphi(\mathbf{x}, -\mathbf{k})$, and that $\sup_{\mathbf{k}\in K} |C(\mathbf{k})| < \infty$ for every compact subset $K \subset \mathbb{R}^3\backslash(\mathscr{E} \cup \{0\})$. Then $\Omega^\pm$ exist, Ran $\Omega^+ =$ Ran Ω^-, and $S = (\Omega^-)^*\Omega^+$ is given by

$$(Sf)(x) = f(x) + \int_{\omega\in S^2} \int \beta(k, \Omega)\hat{f}(|\mathbf{k}|\omega)e^{+i\mathbf{k}\cdot\mathbf{x}}\, d^3k\, d\Omega(\omega)$$

where

$$\beta(k, \Omega) = i\pi^{-1}\gamma(k, \Omega)$$

The details of the proof, which are very similar to those of Theorem XI.69, are left to the reader (Problem 96). However, since the proof provides such a graphic picture of scattering and one which is so similar to that in certain physics textbook presentations, we sketch some of the intermediate steps. Let $g \in C_0^\infty(\mathbb{R}^3\backslash(\mathscr{E} \cup \{0\}))$ and

$$\psi(\mathbf{x}) = \int g(\mathbf{k})\varphi(\mathbf{x}, \mathbf{k})\, d^3k$$

Then, as in the central case,

$$(e^{-iHt}\psi)(\mathbf{x}) = \int g(\mathbf{k})e^{-ik^2t}\varphi(\mathbf{x}, \mathbf{k})\, d^3k$$

By (154) and the dominated convergence theorem, $\|e^{-itH}\psi - \eta_t\| \to 0$ as $t \to \pm\infty$ where

$$\eta_t(\mathbf{x}) = \int g(\mathbf{k})e^{-ik^2t}[e^{i\mathbf{k}\cdot\mathbf{x}} - \gamma(\mathbf{k}, \hat{x})x^{-1}e^{ikx}]\, d^3k$$

The point is that as $t \to -\infty$, the second term goes to zero by an extension of Lemma 3 of Section 3 so that $\|e^{-itH}\psi - e^{-itH_0}[(2\pi)^{3/2}\hat{g}]\| \to 0$ as $t \to -\infty$. As $t \to +\infty$, both terms contribute, and we have both the original wave and a "scattered" wave.

XI.9 Long-range potentials

Both the classical and quantum-mechanical scattering theories that we have developed depend on estimates whose proofs break down when the potentials have r^{-1} falloff. From what we have done so far, it is not clear whether the results could be pushed through for long range potentials with more work on the estimates, but one consequence of what we do in this section is that, in fact, the unmodified theories do not extend further; for example, using Theorem XI.71 below, one can prove (Problem 99) that

$$\text{w-lim}_{t\to\pm\infty} e^{it(-\Delta - r^{-1})}e^{it\Delta} = 0 \tag{155}$$

so that the strong limit does not exist.

In this section we shall first discuss briefly the classical and quantum Coulomb problems and then systematically develop the general long-range case.

At first sight, the scattering theory for classical Coulomb forces seems to be in fine shape. The solutions of

$$\ddot{\mathbf{r}} = -r^{-2}(\mathbf{r}/r)$$

are well known in closed form. The quantities $\ell = \dot{\mathbf{r}} \times \mathbf{r}$ and $E = \frac{1}{2}|\dot{\mathbf{r}}|^2 - r^{-1}$ are conserved. Picking polar coordinates in the plane orthogonal to ℓ, the orbits are given by

$$r(\theta)^{-1} = \ell^{-2}[1 + \sqrt{1 + E\ell^2}\cos(\theta - \theta_0)]$$

This describes an ellipse (or circle) if $E < 0$, a parabola if $E = 0$, and one branch of a hyperbola if $E > 0$. The hyperbolic orbits are clearly the ones one should try to associate with a scattering theory. There are straight line asymptotes to the hyperbolas, which means that the orbit in x space is asymptotic to free orbits. Moreover, the velocity clearly has a limiting direction as $t \to \pm\infty$ and by the fact that $r \to \infty$ and $v = \sqrt{2E + 2r^{-1}}$, it has a limiting magnitude also. Thus the *orbit* in phase space is asymptotic to a free orbit. The problem is with the time parametrization of these orbits. Free orbits have $\mathbf{r}_{\text{free}}(t) = \mathbf{c}t + \mathbf{b} + o(1)$. On the other hand, since $\dot{\mathbf{r}}$ has a limit in the interacting case

$$r(t) = \mathbf{c}t + o(t)$$

as $t \to \infty$. We can further analyze the $o(t)$ term in this expansion by using

$$\frac{1}{\sqrt{2}}\left|\frac{d\mathbf{r}}{dt}\right| = \sqrt{E + r^{-1}} = \sqrt{E}(1 + (2E)^{-1}(ct)^{-1} + o(t^{-1}))$$

to obtain

$$\mathbf{r}(t) = \mathbf{c}t + \mathbf{d} \ln t + O(1)$$

as $t \to \infty$. This makes it clear that the Coulomb orbits $r(t)$ do not approach $\mathbf{a} + \mathbf{b}t$, but nevertheless the occurrence of asymptotes suggests strongly that some kind of modified scattering theory should work. There is a logarithmic slippage of the physical time parametrization of the Coulomb orbit relative to the physical time parametrization of the free asymptote. Notice that $d \geq 0$ so that the particle on the interacting orbit is moving out *faster* than the corresponding free particle on the asymptote. At first sight, this seems surprising since the potential is attractive; the point is that because the potential is attractive, energy conservation implies that the interacting particle is moving faster than its asymptotic velocity.

The above suggests what we might expect in the quantum theory. In $\lim e^{iHt}e^{-iH_0t}$ we must expect to replace e^{-iH_0t} by $e^{-iH_0s(t)}$ where $s(t) = t + d \ln t$. Moreover, looking at the above, one sees that the constant d should be a function of the energy E, that is, e^{-iH_0t} should be replaced by $\exp[-iH_0 t - if(H_0) \ln t]$ for suitable f. To see what choice we should take for the modified quantum dynamics,

$$U_D(t) = \exp[-itH_0 - if(H_0) \ln t]$$

we note that in applying Cook's method to $\exp(it(H_0 + V))U_D(t)$, we shall have to estimate

$$\|[V - t^{-1}f(H_0)]U_D(t)\varphi\|$$

Now, since $U_D(t)$ is almost e^{-itH_0}, we expect, by Theorem IX.31 and also by stationary phase ideas that for large t, "x" will look like $2pt$ since $m = \frac{1}{2}$ if $H_0 = -\Delta$. Thus $x^{-1}U_D(t)\varphi$ will look like $\frac{1}{2}(pt)^{-1}U_D(t)\varphi$. Thus, to effect the cancellation we choose $f(H_0) = -\frac{1}{2}p^{-1}$, which is also the choice one would make on the basis of the classical solutions. To avoid a singularity at $t = 0$ and accommodate $H = -\Delta - \lambda r^{-1}$ we change things slightly and define

$$H_D(t) = H_0 - \tfrac{1}{2}\lambda(p|t|)^{-1}\theta(|4tH_0| - 1)$$

where $H_0 = -\Delta$ and $\theta(a)$ is the characteristic function of $(0, \infty)$. Let

$$U_D(t) = \exp\left(-i\int_0^t H_D(s)\, ds\right) \tag{156}$$

Notice that in (156) we can regard the integral as an integral of functions of p and then define $U_D(t)$ by the functional calculus as a multiplication operator in momentum space.

Theorem XI.71 Let $H_0 = -\Delta$, $H = -\Delta + V(r)$,

$$V(\mathbf{r}) = -\lambda r^{-1} + V_s(\mathbf{r}), \qquad \mathbf{r} \in \mathbb{R}^3$$

where $V_s(\mathbf{r})$ obeys (45). Then

$$\Omega_D^{\pm} = \operatorname*{s-lim}_{t \to \mp\infty} e^{iHt}U_D(t)$$

exist and define isometries with

$$e^{-iHs}\Omega_D^{\pm} = \Omega_D^{\pm}e^{-iH_0s} \tag{157}$$

Proof We shall prove that

$$\|(H - H_D(t))U_D(t)\varphi\| \in L^1(\pm 1, \pm\infty) \tag{158}$$

for φ in a dense set $\mathscr{D}$ of L^2. From this estimate, the existence of $\Omega_D^{\pm}$ follows. The $\Omega_D^{\pm}$ are isometric since $U_D(t)$ is unitary. (157) follows as in the short-range case if one notes that (Problem 100)

$$\operatorname*{s-lim}_{t \to \pm\infty} U_D(t)^*U_D(t + s) = e^{-iH_0s}$$

For $t > 0$, define

$$\tilde{H}_D(t) \equiv H_D(t) - H_0$$

and, for $t > 1/4p^2$,

$$A_D(t) \equiv \int_0^t \tilde{H}_D(s)\, ds = -\tfrac{1}{2}\lambda p^{-1}[\ln t + \ln(4p^2)]$$

(158) in the case $(1, \infty)$ follows from

$$\|V_s(r) \exp(-iH_0 t - iA_D(t))\varphi\| \in L^1(1, \infty) \tag{159a}$$

and

$$\|[-\lambda r^{-1} - \tilde{H}_D(t)] \exp(-iH_0 t - iA_D(t))\varphi\| \in L^1(1, \infty) \tag{159b}$$

(159a) holds for those φ with $\hat{\varphi} \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$ by an elementary modification (Problem 101) of the stationary phase method of Theorem XI.16. Let

$$\eta(x, t) = \exp(ix^2/4t) \exp(i\lambda t(2x)^{-1} \ln(x^2/t))$$

and for $\hat{\varphi} \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$, define

$$R_\varphi(x, t) = U_D(t)\varphi(x) - (2it)^{-3/2}\eta(x, t)\hat{\varphi}(x/2t)$$

We shall show that R_φ satisfies

$$|R_\varphi(x, t)| \leq C(\ln|t|)^\mu t^{-5/2}[1 + (x/t)^2]^{-m} \tag{160}$$

for all $|t| > 2$, any integer m, and suitable constants C and μ depending only on m and φ, and that (160) implies (159b).

We first note that (160) implies that

$$\lim_{t\to\infty} \|U_D(t)\varphi - (2it)^{-3/2}\eta(x, t)\hat{\varphi}(x/2t)\|_2 = 0 \tag{161}$$

for $\hat{\varphi} \in C_0^\infty$ and so for all φ. This is an analogue of (IX.33) and will be very relevant for the physical interpretation of $\Omega_D^\pm$ discussed below.

Let $\varphi_1 = (p^{-1}\hat{\varphi})^\vee$. Then for t sufficiently large

$$\begin{aligned}[(\lambda r^{-1} + \tilde{H}_D(t))U_D(t)\varphi](x) &= (\lambda x^{-1}U_D(t)\varphi)(x) - \lambda(2t)^{-1}(U_D(t)\varphi_1)(x) \\ &= \lambda x^{-1}R_\varphi(x, t) - \lambda(2t)^{-1}R_{\varphi_1}(x, t)\end{aligned}$$

since there is exact cancellation between the terms $\lambda x^{-1}\eta(x, t)\hat{\varphi}(x/2t)$ and $\lambda(2t)^{-1}\eta(x, t)\hat{\varphi}_1(x/2t)$. Now, by (160),

$$\|\lambda x^{-1}R_\varphi(x, t)\|^2 \le t^{-4}(\ln|t|)^{2\mu}$$

and similarly for the φ_1 term. Thus (159) follows if we can prove the estimate (160).

To prove (160), define $\varphi_C(x, t)$ by

$$\varphi_C(x, t) = [e^{-iA_D(t)}\varphi](x)$$

so that for t sufficiently large,

$$\hat{\varphi}_C(k, t) = \exp[\tfrac{1}{2}i\lambda k^{-1}\ln(4k^2t)]\hat{\varphi}(k)$$

Since $\hat{\varphi} \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$, we see that $\hat{\varphi}_C(\cdot, t) \in \mathscr{S}(\mathbb{R}^3)$, and for any norm $\|\cdot\|_\alpha$ on $\mathscr{S}$ and all t with $|t| > 2$,

$$\|\hat{\varphi}_C(\cdot, t)\|_\alpha \le C_\alpha \ln(|t|)^{\nu(\alpha)}$$

and thus

$$\|\varphi_C(\cdot, t)\|_\alpha \le D_\alpha \ln(|t|)^{\mu(\alpha)} \tag{162}$$

since $\hat{}$ is a homeomorphism of $\mathscr{S}$ to $\mathscr{S}$. Now we just follow the proof of Theorem IX.31: Using

$$(U_D(t)\varphi)(x) = (4\pi it)^{-3/2}\int e^{i(x-y)^2/4t}\varphi_C(y, t)\,dy$$

and

$$e^{i(x-y)^2/4t} = e^{ix^2/4t}e^{-ix\cdot y/2t}e^{iy^2/4t}$$

we see that

$$R_\varphi(x, t) = (4\pi it)^{-3/2}e^{ix^2/4t}\int e^{-ix\cdot y/2t}(e^{iy^2/4t} - 1)\varphi_C(y, t)\,dy \tag{163}$$

Using $|e^{iy^2/4t} - 1| \le |y^2/4t|$ and (162), we see that

$$|R_\varphi(x, t)| \le C|t|^{-5/2}\ln(|t|)^\mu$$

Similarly, from (163) and an integration by parts, we see that

$$\begin{aligned}\left|\left(\frac{x}{t}\right)^{2m}R_\varphi(x, t)\right| &\le |t|^{-3/2}\left|\int (-\Delta_y)^m[e^{-ix\cdot y/2t}](e^{iy^2/4t} - 1)\varphi_C(y, t)\,dy\right| \\ &\le |t|^{-3/2}\int |(-\Delta_y)^m[(e^{iy^2/4t} - 1)\varphi_C(y, t)]|\,dy \\ &\le C_m|t|^{-5/2}(\ln|t|)^{\mu(m)}\end{aligned}$$

so that

$$(1 + (x/t)^2)^{2m}|R_\varphi(x, t)| \le C_m|t|^{-5/2}(\ln|t|)^\mu$$

which proves (160). ∎

Before turning to the physical interpretation of $\Omega_D^\pm$, we note two consequences of their existence:

Corollary 1 Suppose that $V_s(\mathbf{r}) \to 0$ at ∞ as well as obeying (45). Then $\sigma_{ac}(H) = [0, \infty)$ where $H = -\Delta - \lambda|\mathbf{r}|^{-1} + V_s(r)$.

Corollary 2 If $\lambda \neq 0$ and H is given as above, the ordinary wave operators $\Omega^\pm(H, H_0)$ do not exist.

Corollary 1 is the standard consequence of (157). Corollary 2 is left to the reader (Problem 99).

We now turn to the physical interpretation of $\Omega_D^\pm$. Let $\psi = \Omega_D^+\varphi$ and define $\psi_t = e^{-iHt}\psi, \varphi_t^{(0)} = e^{-iH_0t}\varphi, \varphi_t^{(D)} = U_D(t)\varphi$. It is not true, as it would be in the short-range case, that $\|\varphi_t^{(0)} - \psi_t\| \to 0$ as $t \to -\infty$. Rather

$$\|\varphi_t^{(D)} - \psi_t\| \to 0 \qquad \text{as} \quad t \to -\infty$$

However, by (161) and (IX.33), we have that

$$\|\eta_t\varphi_t^{(0)} - \varphi_t^{(D)}\| \to 0 \qquad \text{as} \quad t \to \pm\infty$$

and

$$\|\gamma_t\hat{\varphi}_t^{(0)} - \hat{\varphi}_t^{(D)}\| = 0 \qquad \text{all } t$$

for suitable fixed functions $\eta_t(x)$ and $\gamma_t(k)$ of magnitude one. Thus, as $t \to -\infty$,.

$$\int \left| |\varphi_t^{(0)}(x)|^2 - |\psi_t(x)|^2 \right| dx \to 0$$

$$\int \left| |\hat{\varphi}_t^{(0)}(p)|^2 - |\hat{\psi}_t(p)|^2 \right| dp \to 0$$

Therefore, even though ψ_t is not an asymptotically free wave function, *its probability distributions* for both position and momentum approach those of the free wave function $\varphi_t^{(0)}$ as $t \to -\infty$. A similar statement holds as $t \to \infty$. In this sense the motion is "asymptotically free."

One can prove that $\Omega_D^{\pm}$ are complete if one makes stronger hypotheses:

Theorem XI.72 Suppose that

(i) V_s is $-\Delta$-bounded with relative bound $\alpha < 1$.
(ii) $V_s(H_0 + 1)^{-m-1}$ is trace class for some m.

Then $\Omega_D^{\pm}$ are complete in the sense that

$$\text{Ran } \Omega_D^+ = \text{Ran } \Omega_D^- = \mathscr{H}_{\text{ac}}(H)$$

This result can be proven by combining the reference in the Notes with Problem 102. We also remark that multichannel modified wave operators exist; see the Notes. Using the methods of Section 17, Enss has proven strong versions of this result. It seems likely that multichannel analogues will also be proven.

In the remainder of this section, we wish to discuss scattering theory for more general long-range potentials than Coulomb potentials. This general theory will illuminate the choice of $U_D(t)$.

Let us first consider the classical case. Suppose that $\mathbf{F} = -\nabla V$ with

$$\lim_{x \to \infty} V(\mathbf{x}) = 0 \tag{164a}$$

$$|\mathbf{F}(\mathbf{x})| \leq k(1 + x)^{-1-\alpha} \tag{164b}$$

$$|\partial F_i(\mathbf{x})/\partial x_j| \leq k(1 + x)^{-2-\alpha} \tag{164c}$$

where $\alpha > 0$. Of course, if $\alpha > 1$, we are in the short-range case of Section 2, so we suppose $\alpha < 1$. For convenience, we suppose that α^{-1} is not an integer.

We shall also suppose occasionally that F is "almost central" in the sense that for some $\varepsilon > 0$,

$$|\mathbf{F}_\perp(\mathbf{x})| \leq k(1 + x)^{-2-\varepsilon} \tag{165}$$

where $\mathbf{F}_\perp(\mathbf{x}) = \mathbf{F}(\mathbf{x}) - \mathbf{F}_\parallel(\mathbf{x})$ and $\mathbf{F}_\parallel(\mathbf{x}) = x^{-2}(\mathbf{x} \cdot \mathbf{F}(\mathbf{x}))\mathbf{x}$.

As in the short-range case, we consider

$$\dot{\mathbf{x}}(t) = \mathbf{p}(t), \qquad \dot{\mathbf{p}}(t) = -\nabla V, \qquad \mathbf{p}(0) = \mathbf{p}_0, \qquad \mathbf{x}(0) = \mathbf{x}_0 \tag{166}$$

and define

$$\Sigma_\pm = \Big\{ \langle \mathbf{x}_0, \mathbf{p}_0 \rangle \in \mathbb{R}^6 \Big| V(\mathbf{x}_0) + \tfrac{1}{2}p_0^2 > 0 \text{ and the solution } \mathbf{x}(t) \text{ of (166) obeys } \overline{\lim_{t \to \mp\infty}} |\mathbf{x}(t)| = \infty \Big\}$$

As in Section 2, one can show (Problem 103) that $\Sigma_+ = \Sigma_-$ almost everywhere and that for $\langle \mathbf{x}_0, \mathbf{p}_0 \rangle \in \Sigma_\pm$ we have, for some $c > 0$,

$$|\mathbf{x}(t)| \geq c|t| - d \tag{167}$$

for all t with $\mp t \geq 0$.

Theorem XI.73 Let $\mathbf{F}$ and V obey (164).

(a) Let $\langle \mathbf{x}(t), \mathbf{p}(t) \rangle$ be a solution of (166) with initial data in Σ_+. Then

$$\lim_{t \to -\infty} \mathbf{p}(t) \equiv \mathbf{p}_{\text{in}}$$

exists. Moreover, $\mathbf{p}(t) - \mathbf{p}_{\text{in}} = O(|t|^{-\alpha})$ as $t \to -\infty$ and every value of $\mathbf{p}_{\text{in}} \neq 0$ occurs.

(b) If $\mathbf{x}_1(t)$, $\mathbf{x}_2(t)$ are two solutions with $\lim_{t \to -\infty} (\mathbf{p}_1(t) - \mathbf{p}_2(t)) = 0$, then

$$\mathbf{a} \equiv \lim_{t \to -\infty} (\mathbf{x}_1(t) - \mathbf{x}_2(t))$$

exists. Moreover, $|\mathbf{x}_1(t) - \mathbf{x}_2(t) - \mathbf{a}| = O(|t|^{-\alpha})$ as $t \to -\infty$, and for given $\mathbf{p}_{\text{in}} \neq 0$ and associated $\mathbf{x}_1$, every value of $\mathbf{a}$ occurs. If $\mathbf{a} = 0$, then $\mathbf{x}_2 = \mathbf{x}_1$ for all t; and if $\mathbf{a} = \mathbf{p}_{\text{in}} t_0$, then $\mathbf{x}_2(t) = \mathbf{x}_1(t - t_0)$.

(c) Suppose moreover that (165) holds. Then for any vector, $\mathbf{w}$ with $\mathbf{w} \cdot \mathbf{p}_{\text{in}} = 0$,

$$\lim_{t \to -\infty} \mathbf{x}(t) \cdot \mathbf{w} \equiv \alpha(\mathbf{w})$$

exists and $\mathbf{x}(t) \cdot \mathbf{w} - \alpha(\mathbf{w}) = O(|t|^{-\delta})$ where $\delta = \min\{\varepsilon, \alpha\}$. Every linear functional α on $\{\mathbf{w} | \mathbf{w} \cdot \mathbf{p}_{in} = 0\}$ occurs as one runs through all $\mathbf{x}$ with given $\mathbf{p}_{in} \neq 0$.

Proof Let $\langle x(t), p(t) \rangle$ be a solution with initial data in Σ_+. By (164b) and (167),

$$|F(x(t))| \leq k(1 + |x(t)|)^{-1-\alpha} \leq C_1(1 + |t|)^{-1-\alpha}$$

so that

$$\lim_{t \to -\infty} p(t) = p_0 + \lim_{t \to -\infty} \int_0^t F(x(s))\, ds$$

exists and we have $p(t) - p_{in} = O(|t|^{-\alpha})$. We defer the proof that every value of $p_{in} \neq 0$ occurs.

Let x_1, x_2 be two solutions with the same value of p_{in}. Let $\Delta(t) = x_1(t) - x_2(t)$. Then

$$|\dot{\Delta}(t)| = |p_1(t) - p_2(t)| \leq \int_{-\infty}^t |F(x_1(s)) - F(x_2(s))|\, ds$$

since $p_i(t) = p_{in} + \int_{-\infty}^t F(x_i(s))\, ds$. Now, by (164c) and (167),

$$|F(x_1(t) - F(x_2(t))| \leq C_2 |\Delta(t)|(1 + |t|)^{-2-\alpha}$$

so that

$$|\dot{\Delta}(t)| \leq \int_{-\infty}^t |\Delta(s)|(1 + |s|)^{-2-\alpha}\, ds \tag{168}$$

Now suppose that $|\Delta(t)| \leq C_\gamma |t|^\gamma$, $\alpha < \gamma \leq 1$ for $t \leq -1$. Then by (168), $|\dot{\Delta}(t)| \leq C(1 + \alpha - \gamma)^{-1} |t|^{-1-\alpha+\gamma}$ so that

$$|\Delta(t)| = \left| \Delta(-1) + \int_{-1}^t \dot{\Delta}(s)\, ds \right| \leq C'_\gamma |t|^{\gamma-\alpha}$$

Note that $|\Delta(t)| \leq C|t|$. So, using the above N times, where N is chosen so that $\alpha N < 1$, $\alpha(N+1) > 1$, we have that $|\Delta(t)| \leq C' |t|^{1-N\alpha}$. Then, by (168), for $t < 0$,

$$|\dot{\Delta}(t)| \leq C((N+1)\alpha)^{-1} |t|^{-(N+1)\alpha}$$

so that $\lim_{t \to -\infty} \Delta(t) = \Delta(0) + \lim_{t \to -\infty} \int_0^t \dot{\Delta}(s)\, ds$ exists. This means that $\Delta(t)$ is bounded, and thus by (168), $\Delta(t) - a = O(|t|^{-\alpha})$. Again we defer the proof that every a occurs.

If $a = 0$, then $\Delta(t) \to 0$ as $t \to -\infty$. As a result, by (168), we can write for $t < 0$

$$|\Delta(t)| \leq (2 + \alpha)^{-1}(1 + \alpha)^{-1}(1 + |t|)^{-\alpha} \sup_{-\infty \leq s < t} |\Delta(s)|$$

Choosing t so that $(2 + \alpha)^{-1}(1 + \alpha)^{-1}(1 + |t|)^{-\alpha} < 1$, we conclude that $\Delta(s) = 0$ for $s \leq t$ so that $\Delta(t) = 0$ for all t by local uniqueness.

Given t_0 and $x_1(t)$, it is easily seen that $x_3(t) \equiv x_1(t - t_0)$ obeys $\dot{x}_3(t) \to p_{in}$ and $x_1(t) - x_3(t) = \int_{t-t_0}^t \dot{x}_1(s)\, ds \to p_{in} t_0$. By the uniqueness just proven, any x_2 with $\dot{x}_2 \to p_{in}$ and $x_1 - x_2 \to p_{in} t_0$ is equal to x_3.

Now suppose that (165) holds and let $w \cdot p_{in} = 0$. Suppose that $|w \cdot F(x(t))| \leq C|t|^{-\gamma}$ where $1 < \gamma < 2$. Then, since

$$w \cdot p(t) = \int_{-\infty}^t w \cdot F(x(s))\, ds \tag{169}$$

$$w \cdot x(t) = w \cdot x(0) + \int_0^t (p(s) \cdot w)\, ds$$

we have

$$|w \cdot x(t)| \leq C_2(1 + |t|)^{2-\gamma}$$

So, by (167),

$$|w \cdot x(t)|\, |x(t)|^{-1} \leq C_4(1 + |t|)^{1-\gamma}$$

As a result, using

$$|a \cdot F(x(s))| \leq |F_\perp(x(s))|\, |a| + \frac{|a \cdot x(s)|}{|x(s)|}\, |F(x(s))|$$

we have by (164b) and (165),

$$|w \cdot F(x(t))| \leq (\text{const})[(1 + |t|)^{-2-\varepsilon} + (1 + |t|)^{-\gamma-\alpha}]$$

By repeating this process, beginning with $\gamma = 1 + \alpha$,

$$|w \cdot F(x(t))| \leq (\text{const})(1 + |t|)^{-2-\delta}$$

where $\delta = \min(\varepsilon, \alpha)$. Thus, using (169), we have that $w \cdot p(t) = O(|t|^{-1-\delta})$, so $w \cdot x(t)$ has a limit $\alpha(w)$ and $w \cdot x(t) - \alpha(w) = O(|t|^{-\delta})$.

Finally, we return to the question of existence, that is, that every $\mathbf{p}_{in} \neq 0$ and $\mathbf{a}$ occurs; this will automatically imply that every α occurs for the linear map $w \mapsto \alpha(w)$. Obviously, it suffices to construct an auxiliary function $\mathbf{z}(\mathbf{p}, t)$ so that $\lim_{t \to -\infty} \dot{\mathbf{z}}(\mathbf{p}, t) = \mathbf{p}$ and then for any $\mathbf{a}$, a solution $\mathbf{x}(t)$ with $\lim_{t \to -\infty} (\mathbf{x}(t) - \mathbf{z}(\mathbf{p}, t)) = \mathbf{a}$ and $\lim_{t \to -\infty} \dot{\mathbf{x}}(t) = \mathbf{p}$. $\mathbf{z}$ will replace the elementary $\mathbf{p}t$ used in the short-range case. Once, we have the "right" $\mathbf{z}(\mathbf{p}, t)$, we shall construct the solution $\mathbf{x}$ by the contraction mapping theorem as in the short-range case.

How can one find a good choice for $\mathbf{z}(\mathbf{p}, t)$? To get an approximate value of $\dot{\mathbf{z}}$ which will go to $\mathbf{p}$ as $t \to -\infty$, we shall try to integrate from $t = -\infty$.

However, we shall not be able to get $\mathbf{z}$ by integrating $\dot{\mathbf{z}}$ from $-\infty$ since $\dot{\mathbf{z}}$ will approach $\mathbf{p}$ only as a power $|t|^{-\alpha}$ with $\alpha < 1$. Thus we shall integrate $\dot{\mathbf{z}}$ from $t = 0$. Therefore we define $\mathbf{z}_n(\mathbf{p}, t)$ inductively by

$$\mathbf{z}_0(\mathbf{p}, t) = \mathbf{p}t$$

$$\dot{\mathbf{z}}_n(\mathbf{p}, t) = \mathbf{p} + \int_{-\infty}^{t} \mathbf{F}(\mathbf{z}_{n-1}(\mathbf{p}, s))\, ds$$

$$\mathbf{z}_n(\mathbf{p}, t) = \int_0^t \dot{\mathbf{z}}_n(\mathbf{p}, s)\, ds$$

We take $z(p, t) = z_N(p, t)$ where $N = [1/\alpha]$, the integral part of $1/\alpha$. Clearly, for any fixed $p \neq 0$ and $t \leq 0$,

$$|z_n(p, t)| \geq c|t| - d \tag{170}$$

for $n = 0, \ldots, N$ and some $c > 0$. Moreover, by a simple inductive argument of the type we have already used,

$$|z_n(p, t) - z_{n-1}(p, t)| \leq Kt^{1-n\alpha} \tag{171}$$

for $n = 1, \ldots, N$. Now, if x obeys

$$\ddot{x}(t) = F(x(t))$$

$$x(t) - z_N(p, t) - a \to 0$$

$$\dot{x}(t) - \dot{z}_N(p, t) \to 0$$

then $y(t) = x(t) - z_N(p, t) - a$ obeys

$$y(t) = \int_{-\infty}^{t} \int_{-\infty}^{w} [F(z_N(p, s) + a + y(s)) - F(z_{N-1}(p, s))]\, ds\, dw \tag{172}$$

Conversely, solutions of (172) yield solutions of Newton's equation with the desired asymptotic behavior. Given (164c), (170), and (171), one can mimic the contraction mapping method of Section 2 (Problem 104) and find solutions of (172) and to obtain the existence result needed to complete the proof. ∎

What is the physical interpretation of this theorem? Consider the case where both (164) and (165) hold. Then, given $\mathbf{p}_{\text{in}} \neq 0$ and $\mathbf{b}_{\text{in}}$ perpendicular to $\mathbf{p}_{\text{in}}$, there is a one-parameter family of solutions x_s with

$$\dot{\mathbf{x}}_s(t) \to \mathbf{p}_{\text{in}}$$

$$\mathbf{x}_s(t) - \mathbf{p}_{\text{in}}(\mathbf{p}_{\text{in}} \cdot \mathbf{x}(s))p_{\text{in}}^{-2} \to \mathbf{b}_{\text{in}}$$

as $t \to -\infty$. They differ only by time parameterization, that is, $x_s(t) = x_0(t - s)$. Thus, if $\langle \mathbf{x}_s(0), \dot{\mathbf{x}}_s(0) \rangle \in \Sigma_-$ (and this will happen for almost all $\mathbf{p}_{\text{in}}$, $\mathbf{b}_{\text{in}}$; see Problem 105), $\lim_{t\to\infty} \dot{\mathbf{x}}_s(t) \equiv \mathbf{p}_{\text{out}}$ and

$$\lim_{t\to\infty} [\mathbf{x}_s(t) - \mathbf{p}_{\text{out}}(\mathbf{p}_{\text{out}} \cdot \mathbf{x}(s))p_{\text{out}}^{-2}] \equiv \mathbf{b}_{\text{out}}$$

are independent of s. As a result, one has a natural definition of a map

$$\tilde{S}\colon \langle \mathbf{p}_{\text{in}}, \mathbf{b}_{\text{in}} \rangle \to \langle \mathbf{p}_{\text{out}}, \mathbf{b}_{\text{out}} \rangle$$

As in the short-range case, if the force is central, $\mathbf{b}_{\text{out}}$ is completely determined by $\mathbf{p}_{\text{out}}$ and conservation of angular momentum, so that S is described by giving a single scattering angle as a function of $\mathbf{p}_{\text{in}}$ and $\mathbf{b}_{\text{in}}$. The point is that we can see precisely what is lost in going from short-range to long-range; namely in the long-range case, there is no finite time delay. In fact, one can show (Problem 106) that if $V_\varepsilon(x)$ is some short-range modification of V, say $V_\varepsilon(x) = e^{-\varepsilon x^2}V(x)$, then as $\varepsilon \to 0$ the part of the scattering operator given by $\tilde{S}_\varepsilon$ converges to the $\tilde{S}$ defined above. Typically the time delays will diverge as $\varepsilon \to 0$ if V is truely long-range.

The above discussion suggests that the problem of long-range quantum scattering should be connected with infinite, energy-dependent phases since classical time delay is analogous to the phase of the quantum scattering operator. The changes from the ordinary to the modified dynamics can be viewed precisely as an infinite energy dependent adjustment of phase. Unfortunately, the above formulation does not have a quantum generalization because the map $\langle p, a \rangle \to z_N(p, t) + a$ for fixed t is *not* in general a canonical transformation, so that it will not in general correspond in quantum mechanics to a unitary operator. One can sometimes construct approximate solutions $\tilde{z}(p, a, t)$ so that $\langle p, a \rangle \to \tilde{z}(p, a, t)$ is a canonical transformation for each t and so that there is a solution $x(p, a, t)$ of (166) with $|x - \tilde{z}| + |\dot{x} - \dot{\tilde{z}}| \to 0$ as $t \to -\infty$ and $\dot{\tilde{z}}(p, a, t) \to p$, $\tilde{z}(p, a, t) - \tilde{z}(p, b, t) \to a - b$ as $t \to -\infty$. It is the analogue of this classical construction that we shall follow in the quantum case below. One can reprove Theorem XI.73 by following the arguments that we shall give in the quantum case below in the classical case, and thereby one can obtain a proof with an approximate dynamics which *is* given by a canonical transformation; see the reference in the Notes and Problem 107.

Theorem XI.74 Let $V = V_L + V_s$ be a measurable function on $\mathbb{R}^n$ so that V_s obeys (45) and V_L obeys

$$|(D^\alpha V_L)(x)| \leq C(1 + x)^{-|\alpha|-\varepsilon}; \qquad |\alpha| \leq M$$

where $\varepsilon > \frac{1}{2}$ if $M = 1$, $\varepsilon > \frac{1}{5}$ if $M = 2$, and $\varepsilon > 0$ if $M = 3$. Then, there exists a C^∞ function $W(\mathbf{k}, t)$ for $\mathbf{k} \in \mathbb{R}^n \backslash \{0\}$, $t \in \mathbb{R}$, so that

(a) $W(k, s+t) - W(k, t) \to \frac{1}{2}sk^2$ as $t \to \pm\infty$ for each fixed k, s. (173)

(b) For any self-adjoint extension H of $-\frac{1}{2}\Delta + V$ on $C_0^\infty(\mathbb{R}^n)$,

$$\operatorname*{s-lim}_{t \to \mp\infty} e^{iHt} U_D(t) \equiv \Omega_D^\pm$$

exist where $U_D(t) = \exp(-iW(-i\nabla, t))$.

The full proof of this result involves many detailed estimates. We shall not give it here, but will describe several important aspects including the method for constructing W.

The point of (173) is that it implies (Problem 100) that

$$\operatorname*{s-lim}_{t \to \pm\infty} [U_D(t+s)U_D(t)^{-1}] = e^{-isH_0}$$

so that the usual intertwining relation holds:

$$e^{-isH}\Omega_D^\pm = \Omega_D^\pm e^{-isH_0}$$

Of course, one can object that W may not be uniquely determined, and in fact it is not. However, if W and W' are two functions for which (a) and (b) hold and if Ran $\Omega_D^+ = \mathscr{H}_{ac}(H)$, then (Problem 108) there is a measurable function $F(k)$ that is finite a.e. so that

$$(\Omega_D^\pm)' = \Omega_D^\pm e^{iF(-i\nabla)}$$

In particular, Ran Ω_D^+ is independent of W and so asymptotic completeness holds for one choice of W if and only if it holds for any other choice.

In addition, one can show that for any choice of W, the asymptotic *probability distribution* of $U_D(t)f$ in both x and p space is the same as that of $e^{-itH_0}f$. Of course, if $(\Omega_D^\pm)' = \Omega_D^\pm e^{iF_\pm(k)}$, then the kernel of the on-energy-shell S-operators obeys

$$S'(k, k') = S(k, k')e^{i(F_+(k) - F_-(k'))}$$

so that the differential cross sections will also be independent of the choice of W. Unfortunately the "phase" of $S(k, k')$ is not determined until one makes a choice of W. The question of what is the "right phase" is an interesting question which we discuss in the notes.

We now turn to three aspects of the proof of Theorem XI.74: (i) smoothing V_L, (ii) choosing W, (iii) some remarks on the detailed estimates.

Clearly, given V obeying the hypothesis of Theorem XI.74, there will be many decompositions of V into $V_L + V_s$ where V_s obeys (45). The first step is to pick a decomposition such that V_L is C^∞ with derivatives that fall off more and more rapidly at infinity. In fact one can construct such a decomposition with

$$|(D^\alpha V_L)(x)| \leq C_\alpha (1+x)^{-m(|\alpha|)} \tag{174a}$$

for all α where

$$m(1) + m(3) > 4 \tag{174b}$$

and

$$m(\ell) \geq \delta\ell - \varepsilon \tag{174c}$$

$\delta > \frac{1}{2}$. For example (Problem 109), in the case $\varepsilon > 0$, $M = 3$, one can take $m(1) = 1 + \varepsilon$, $m(2) = 2 + \varepsilon$, $m(3) = 3 + \varepsilon$, $m(\ell) = 3 + \varepsilon + \frac{2}{3}(\ell - 3)$ for $\ell > 3$. How does one construct V_L? Begin with a breakup $\tilde{V}_s + \tilde{V}_L = V$. The obvious first guess for V_L would be $f = h * \tilde{V}_L$ where h is in C_0^∞. f is C^∞, but higher derivatives will not automatically fall off since $\tilde{V}_L$ may only be C^1 and $D^\alpha h$ has no "falloff." Somehow even though h is fixed, one wants it to be more and more spread out as $x \to \infty$! To arrange this, one writes $\tilde{V}_L = \sum \tilde{V}_L^{(n)}$ where $\tilde{V}_L^{(n)}$ have support in wider and wider spherical shells which march out to infinity. Then we take $V_L = \sum h_n * \tilde{V}_L^{(n)}$ where the h_n become more and more spread out. To get $V_L - \tilde{V}_L$ short-range, one needs an additional trick. The construction for the case $\varepsilon > 0$, $M = 3$ is outlined in Problem 109.

As we shall explain later, (174b) is critical. It clearly holds in case $M = 3$, $\varepsilon > 0$; and it is the reason that for $\varepsilon > 0$, $M = 3$ always works and we never need a priori information on $D^\alpha V_L$ with $|\alpha| \geq 4$. It also is the reason one needs $\varepsilon > \frac{1}{2}$ (respectively, $\varepsilon > \frac{1}{5}$) if $M = 1$ (respectively, 2). When one goes through the above construction of a new V_L, these values of ε are required to assure (174b) (see Problem 110).

Next, we turn to the construction of W. In applying Cook's method to control the limit $\Omega_D^\pm$ one has to estimate

$$\iint \left(\frac{1}{2}k^2 + V(x) - \frac{\partial W}{\partial t}\right) e^{ik\cdot x - iW(k,t)} \hat{\varphi}(k)\, dx\, dk$$

The short-range piece of V should be controlled as in the short-range case. The long-range case will have to be cancelled in part by $\partial W/\partial t$ as in the Coulomb case. If the method of stationary phase is used, we expect that the

above integral will be concentrated near points where $x = \partial W/\partial k$. Thus, to effect as great a cancellation as possible, one might try to solve

$$V_L\left(\frac{\partial W}{\partial k}\right) + \frac{k^2}{2} = \frac{\partial W}{\partial t} \tag{175}$$

Before discussing exact solutions of this nonlinear partial differential equation, we want to write it in some alternative forms and discuss approximate solutions. It is natural to think of $U_D(t)$ as coming from integrating a time dependent equation with Hamiltonian

$$H(t) = H_0 + f(-i\nabla, t)$$

Clearly, we should choose

$$f(k, t) \equiv \frac{\partial W}{\partial t} - \frac{k^2}{2} \tag{176}$$

If we define $x(k, t) \equiv \partial W/\partial k$, then (175) becomes

$$f(k, t) = V_L(x(k, t)) \tag{177}$$

Now by applying $\partial/\partial k$ to (175), one sees that $x(k, t)$ obeys the differential equation

$$\dot{x}(k, t) = k + \nabla_k V_L(x(k, s)) \tag{178}$$

If we try to choose $W \equiv 0$ for $t = t_0$, then (177) and (178) give the integral equation

$$f(k, t) = V_L\left(kt - kt_0 + \int_{t_0}^{t} \nabla_k f(k, s)\, ds\right) \tag{179}$$

The simplest approximate solution of (179) is to take $t_0 = 0$ and

$$f(k, t) \approx V_L(kt)$$

Using

$$W(k, t) = \tfrac{1}{2}k^2 t + \int_{t_0}^{t} f(k, s)\, ds + \text{const}$$

we see that this approximation leads to the choice of W we used in the Coulomb case. This choice can be used to define modified wave operators for $V_L(x) = |x|^{-\alpha}$, so long as $\alpha > \frac{1}{2}$. For $\alpha < \frac{1}{2}$, it is necessary to try either to solve (175) exactly or go to a higher approximation of (179), for example,

$$f(k, t) \approx V_L\left(kt + \int_0^t s(\nabla V_L)(ks)\, ds\right)$$

This method of higher approximation has been used, but it turns out to require information about more and more derivatives of V_L as $\alpha \to 0$.

The key to the proof of Theorem XI.74 is the construction of *exact* solutions of (175) which result from realizing that it is a standard equation of the advanced theory of classical mechanics, namely the momentum space **Hamilton–Jacobi equation.** We can now give a formal construction of solutions of (175). Let $g(\eta)$ be an arbitrary smooth function on $\mathbb{R}^n$ (or a subset of $\mathbb{R}^n$). Fix t_0 real. Let $X(\eta, t)$ be the solution of Newton's equation

$$\ddot{X}(\eta, t) = -(\nabla V_L)(X(\eta, t))$$

with initial conditions

$$X(\eta, t_0) = g(\eta) \tag{180a}$$

$$\dot{X}(\eta, t_0) = \eta \tag{180b}$$

Suppose that for each fixed t, the map $\eta \mapsto k \equiv \dot{X}(\eta, t)$ is invertible, with inverse function $\eta = N(k, t)$, that is,

$$\dot{X}(N(k, t), t) = k \tag{181}$$

Define

$$x(k, t) = X(N(k, t), t) \tag{182}$$

that is, x is the position at time t of that solution of Newton's equation obeying (180) which has velocity k at time t. We claim that x obeys (178) so that we can recover solutions of (179) by using (176) and (177). To check that x obeys (178), we first differentiate (181) with respect to k and t to obtain

$$\frac{\partial \dot{X}}{\partial \eta}\frac{\partial N}{\partial k} = 1 \tag{183}$$

$$\frac{\partial \dot{X}}{\partial \eta}\frac{\partial N}{\partial t} + \frac{\partial \dot{X}}{\partial t} = 0$$

so that, using $\ddot{X}(\eta, t) = -(\nabla V_L)(X)$, we obtain

$$\frac{\partial \dot{X}}{\partial \eta}\frac{\partial N}{\partial t} = (\nabla V_L)(x) \tag{184}$$

From (182), we obtain

$$\frac{\partial x}{\partial k} = \frac{\partial X}{\partial \eta}\frac{\partial N}{\partial k} \tag{185}$$

From (183)–(185), we see that

$$\frac{\partial N}{\partial t}\frac{\partial X}{\partial \eta} = (\nabla V_L)(x)\frac{\partial x}{\partial k} = \frac{\partial}{\partial k} V_L(x(k, t))$$

so that

$$\dot{x}(k, t) = \frac{\partial X}{\partial t} + \frac{\partial X}{\partial \eta}\frac{\partial N}{\partial t}$$

$$= k + \frac{\partial}{\partial k} V_L(x(k, t))$$

which is (178).

The only "formal" aspect of the above involves the invertibility of $\eta \mapsto \dot{X}(\eta, t)$. By using the asymptotic information on V_L, one can construct a function $W(k, t)$ on $\{\mathbb{R}^n\backslash\{0\}\} \times \mathbb{R}$ such that for any compact $K \subset \mathbb{R}^n\backslash\{0\}$, there is a T_K with W obeying (175) on $K \times \{t \mid |t| > T_K\}$. This is the function W used to construct the generalized wave operators.

Finally, we turn to some aspects of the estimates. The importance of (174b) comes from the fact that when it holds, one can show that W obeys

$$|D_k^\alpha(t^{-1}\,\partial W/\partial k - k)| \leq Ct^{-\beta}, \qquad |\alpha| \leq 1$$

for some $\beta > 0$. This means that for t large the critical points of $x \cdot k - W(k, t)$ that are solutions of

$$x/t = k + t^{-1}(\partial W/\partial k - tk)$$

are unique and are near the short-range critical point $x/t = k$. The other aspect of the detailed estimates that we should mention is that one must push stationary phase methods even further than we do in Theorem XI.15. After rewriting

$$\int u(k)e^{i\omega f(k)}\,dk = \int v(y)e^{i\omega\langle y, Ay\rangle/2}\,dy$$

as we do there and using (43), one must make an expansion of $e^{i\langle k, A^{-1}k\rangle/2\omega}$ in powers of ω^{-1} rather than using the simple estimate used in Theorem XI.15.

XI.10 Optical and acoustical scattering I: Schrödinger operator methods

In this section we present techniques for describing the scattering of classical waves in inhomogeneous media. The methods are geared to linear wave equations and are applicable to acoustic and optical scattering. The basic

physical situation is as follows. Suppose that we have an inhomogeneous medium that looks more and more homogeneous as $x \to \infty$. The propagation of acoustical or optical waves in the medium will be governed by a linear wave equation with nonconstant coefficients because of the inhomogeneity. If the initial disturbance is of finite energy, then as t gets large the waves should propagate out toward infinity. As they do so, they should look more and more like solutions of the corresponding equations with constant coefficients. Thus, we should be able to develop a scattering theory that relates the solutions of the nonconstant coefficient equation to the solutions of the corresponding equation with constant coefficients.

The basic idea in this section is to formulate both the homogeneous and inhomogeneous equations as Hilbert space problems so that we can use the methods developed earlier in this chapter. This will lead us necessarily to the problem of comparing unitary groups on two *different* Hilbert spaces. In the next section we describe another approach to these problems due to Lax and Phillips. To see how the problem of two Hilbert spaces arises, we begin with an example.

Example 1 (acoustical scattering in inhomogeneous media) The propagation of sound waves in a homogeneous medium can be described by specifying at each time t the function $u(x, t)$ which is the difference between the pressure at x and the equilibrium pressure. If one linearizes the nonlinear equations of fluid dynamics about the equilibrium pressure, an approximation that is good for small u, one obtains the wave equation

$$u_{tt}(x, t) = c_0^2\,\Delta u(x, t)$$
$$u(x, 0) = f(x), \qquad u_t(x, 0) = g(x) \tag{186}$$

where f and g are specified by the initial disturbance and c_0 is the velocity of propagation of the pressure waves.

Now, if the medium in which the waves are traveling has a density $\rho(x)$ that varies with position, then the pressure will satisfy the more complicated equation

$$u_{tt}(x, t) = c(x)^2\rho(x)\nabla \cdot \frac{1}{\rho(x)}\nabla u$$
$$u(x, 0) = f(x), \qquad u_t(x, 0) = g(x) \tag{187}$$

where the velocity $c(x)$ will also vary with position since the density does. Suppose that

$$c(x) \to c_0, \qquad \rho(x) \to \rho_0 \tag{188}$$

as $|x| \to \infty$. If this convergence is rapid enough, then we should be able to develop a scattering theory for (186) and (187) since we expect the solutions of (187) to propagate out toward ∞. And, when they are out near infinity, they should look very much like solutions of (186).

We formulate both equations as Hilbert space problems using the ideas in Section X.13. We deal with (186) first. Let $H_0 = -c_0^2\Delta$ on $L^2(\mathbb{R}^3)$ and $B_0 = \sqrt{H_0}$. Denote by $[D(B_0)]$ the closure of $D(B_0)$ in the norm $\|B_0 u\|_2$. Note that $[D(B_0)]$ contains ideal elements that are not in $L^2(\mathbb{R}^3)$ because zero is in $\sigma(B_0)$. Let $\mathscr{H}_0$ be the Hilbert space

$$\mathscr{H}_0 = [D(B_0)] \oplus L^2(\mathbb{R}^3)$$

with norm

$$\|\langle u, v\rangle\|^2 = \|B_0 u\|_2^2 + \|v\|_2^2$$

and define

$$A_0 = i\begin{pmatrix} 0 & I \\ -B_0^2 & 0 \end{pmatrix}, \qquad D(A_0) = D(B_0^2) \oplus D(B_0)$$

where

$$D(B_0^2) = \{u \in [D(B_0)] \mid B_0 u \in D(B_0)\}$$

and we are denoting both B_0 and its extension to $[D(B_0)]$ by B_0. Then A_0 is self-adjoint on $D(A_0)$ and (186) may be reformulated as

$$\begin{aligned} \varphi'(t) &= -iA_0\varphi(t) \\ \varphi(0) &= \varphi_0 \equiv \langle f, g\rangle \end{aligned} \tag{189}$$

for the $\mathscr{H}_0$-valued function $\varphi(t) = \langle u(t), u_t(t)\rangle$. The solution is given by $\varphi(t) = W_0(t)\varphi_0$ where

$$W_0(t) = e^{-iA_0 t} = \begin{pmatrix} \cos B_0 t & B_0^{-1}\sin B_0 t \\ -B_0 \sin B_0 t & \cos B_0 t \end{pmatrix}$$

with the matrix entries defined by the functional calculus. If $\varphi_0 \in D(A_0)$, then $\varphi(t)$ is strongly differentiable and satisfies (189), which implies that the first component $u(t)$ satisfies (186). It will later be convenient to change the inner product on $L^2(\mathbb{R}^3)$ by a fixed constant.

In order to deal with (187), we assume in addition to (188) that

$$0 < \rho_1 \le \rho(x) \le \rho_2 < \infty \qquad \text{for all } x \tag{190a}$$

$$0 < c_1 \le c(x) \le c_2 < \infty \qquad \text{for all } x \tag{190b}$$

If in addition ρ is C^1, then

$$H_1 = -c(x)^2\rho(x)\nabla \cdot \rho(x)^{-1}\nabla$$

is a well-defined operator on $C_0^\infty(\mathbb{R}^3)$. But it is clear that it is not even formally symmetric in the usual L^2 inner product because of the factor $c(x)^2\rho(x)$. However, if we define $L^2_{\rho c}(\mathbb{R}^3)$ to be $L^2(\mathbb{R}^3)$ with the inner product

$$(f, g)_{\rho c} = (f, (c^2\rho)^{-1}g)_{L^2(\mathbb{R}^3)}$$

then in this new inner product H_1 is obviously symmetric on $C_0^\infty(\mathbb{R}^3)$. Notice that, by (190a), $L^2_{\rho c}$ and L^2 are equal as sets; in fact, the norms are equivalent. Associated to H_1 on $C_0^\infty(\mathbb{R}^3) \subset L^2_{\rho c}$ is the quadratic form

$$\begin{aligned} q_1(f, g) = (f, H_1 g)_{\rho c} &= (f, -\nabla \cdot \rho^{-1}\nabla g)_{L^2} \\ &= (\nabla f, \rho^{-1}\nabla g)_{L^2} \end{aligned}$$

The form q_1 is positive and closable by assumption (190a). In fact, since

$$\rho_2^{-1}(\nabla f, \nabla f)_2 \le (\nabla f, \rho^{-1}\nabla f)_2 \le \rho_1^{-1}(\nabla f, \nabla f) \tag{191}$$

the closure of q_1 has form domain $Q(-\Delta)$. Let H_1 be the self-adjoint operator on $L^2_{\rho c}$ corresponding to the closure of q_1 according to Theorem VIII.15. We now proceed as before by defining $B_1 = \sqrt{H_1}$, $[D(B_1)]$ to be the closure of $D(B_1)$ in the norm $\|B_1 u\|_{\rho c}$, and

$$\mathscr{H}_1 = [D(B_1)] \oplus L^2_{\rho c}(\mathbb{R}^3)$$

$$A_1 = i\begin{pmatrix} 0 & I \\ -B_1^2 & 0 \end{pmatrix}$$

Then A_1 is self-adjoint on $D(B_1^2) \oplus D(B_1)$ and generates

$$W_1(t) = \begin{pmatrix} \cos B_1 t & B_1^{-1}\sin B_1 t \\ -B_1 \sin B_1 t & \cos B_1 t \end{pmatrix}$$

As before, if $\varphi_0 \in D(A_1)$, then $u(t)$, the first component of

$$\varphi(t) = W_1(t)\varphi_0$$

satisfies (187). Notice that the above construction of H_1 did not require any regularity on $c(x)$ or $\rho(x)$. However, if they are both smooth, then H_0 and H_1 are both essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ (see Problem 66).

In order to develop a scattering theory for (187), we must compare $W_1(t)$ on $\mathscr{H}_1$ to $W_0(t)$ on $\mathscr{H}_0$. The domains of B_0 and B_1 are both equal to $Q(-\Delta)$; and, by (191), we have

$$\rho_2^{-1}\|B_0 u\|_2^2 \le \|B_1 u\|_{\rho c}^2 \le \rho_1^{-1}\|B_0 u\|_2^2 \tag{192}$$

so $\mathscr{H}_0$ and $\mathscr{H}_1$ are equal as sets, but they have different (though equivalent) inner products. If we restrict ourselves to one inner product, then one of the two groups will not be unitary. We are thus in a situation where it is natural to apply the two Hilbert space formalism outlined in Section 3.

In order to study the kind of situation described in the above example, we formulate the problem abstractly. Let H_0 and H_1 be nonnegative self-adjoint operators on Hilbert spaces $\mathscr{K}_0$ and $\mathscr{K}_1$. To make the presentation easier we shall assume that H_0 and H_1 have no point spectrum at zero; the general case is treated in the references given in the Notes. We want to develop a scattering theory for the two equations

$$u_0''(t) = -H_0 u_0(t)$$
$$u_1''(t) = -H_1 u_1(t)$$

when we are given a "natural" unitary identification operator $V: \mathscr{K}_0 \to \mathscr{K}_1$. Let $\mathscr{H}_0$ and $\mathscr{H}_1$ be the Hilbert spaces

$$\mathscr{H}_0 = [D(B_0)] \oplus \mathscr{K}_0$$
$$\mathscr{H}_1 = [D(B_1)] \oplus \mathscr{K}_1$$

constructed as in the example with $B_k = \sqrt{H_k}$ and with norms

$$\|\langle u, v\rangle\|_0^2 = \|B_0 u\|_{\mathscr{K}_0}^2 + \|v\|_{\mathscr{K}_0}^2$$
$$\|\langle u, v\rangle\|_1^2 = \|B_1 u\|_{\mathscr{K}_1}^2 + \|v\|_{\mathscr{K}_1}^2$$

The solutions of the above equations are given by

$$\begin{pmatrix} u_k(t) \\ u_k'(t) \end{pmatrix} = W_k(t) \begin{pmatrix} u_k(0) \\ u_k'(0) \end{pmatrix}$$

where

$$W_k(t) = \begin{pmatrix} \cos B_k t & B_k^{-1} \sin B_k t \\ -B_k \sin B_k t & \cos B_k t \end{pmatrix}$$

As in the example, we denote the generator of $W_k(t)$ by A_k.

Our plan of attack is to reduce the questions of existence and completeness of the wave operators for $W_0(t)$, $W_1(t)$ to the same questions for $V^{-1}H_1 V$ and H_0 on $\mathscr{K}_0$. In this way the two Hilbert space problem is reduced to a single Hilbert space problem involving operators similar to the Schrödinger operators which we have already studied. We shall later show how one can stay in the two Hilbert space setting and apply Theorem XI.13 (see Example 1, revisited). We use without comment the notation and terminology of two Hilbert space scattering introduced in Section 3.

We begin by choosing an identification operator J between $\mathscr{H}_0$ and $\mathscr{H}_1$ which is mathematically convenient but physically unnatural. Later we shall show that under certain circumstances, usually fulfilled in applications, other more natural identification operators are (asymptotically A_0-) equivalent to J. We define $J: \mathscr{H}_0 \to \mathscr{H}_1$ by

$$J: \langle u, v\rangle \mapsto \langle B_1^{-1} V B_0 u, Vu\rangle$$

Theorem XI.75 Let $\mathscr{K}_k$, $\mathscr{H}_k$, H_k, B_k, A_k, $k = 0, 1$, and V and J be as defined above. Suppose that the wave operators $\Omega^{\pm}(V^{-1}B_1 V, B_0)$ exist (respectively, exist and are complete) on $\mathscr{K}_0$. Then the generalized wave operators $\Omega^{\pm}(A_1, A_0; J)$ exist (respectively, exist and are complete) and are partial isometries from $\mathscr{H}_0$ to $\mathscr{H}_1$ with initial space $P_{ac}(A_0)\mathscr{H}_0$.

Proof Since

$$\begin{aligned} \|J\langle u, v\rangle\|_{\mathscr{H}_1}^2 &= \|B_1(B_1^{-1}VB_0)u\|_{\mathscr{K}_1}^2 + \|Vv\|_{\mathscr{K}_1}^2 \\ &= \|B_0 u\|_{\mathscr{K}_0}^2 + \|v\|_{\mathscr{K}_0}^2 \\ &= \|\langle u, v\rangle\|_{\mathscr{H}_0}^2 \end{aligned}$$

J is unitary and thus $\Omega^{\pm}(A_1, A_0; J)$ are partial isometries when they exist. The proof of the main statement of the theorem relies on the factorization

$$\frac{d^2}{dt^2} + B^2 = \left(\frac{d}{dt} - iB\right)\left(\frac{d}{dt} + iB\right)$$

so that if u obeys $u'' = -B^2 u$, then $f_{\pm} = u' \pm iBu$ obey $df_{\pm}/dt = \pm iBf_{\pm}$. To make the decomposition precise, we define

$$T_k = \frac{1}{\sqrt{2}} \begin{pmatrix} B_k & i \\ B_k & -i \end{pmatrix}$$

Then, by the parallelogram law, T_k is a unitary map of $\mathscr{H}_k$ onto $\mathscr{K}_k \oplus \mathscr{K}_k$ and

$$T_k A_k T_k^{-1} = \begin{pmatrix} B_k & 0 \\ 0 & -B_k \end{pmatrix}$$

Thus

$$T_k W_k(t) T_k^{-1} = \begin{pmatrix} e^{-iB_k t} & 0 \\ 0 & e^{iB_k t} \end{pmatrix} \equiv \tilde{W}_k(t)$$

Further, by multiplying out the matrices, one finds

$$T_1 J T_0^{-1} = \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} \equiv \tilde{V}$$

as a map from $\mathscr{K}_0 \oplus \mathscr{K}_0$ to $\mathscr{K}_1 \oplus \mathscr{K}_1$. Moreover, by Problem 112,

$$T_0 P_{ac}(A_0) = \begin{pmatrix} P_{ac}(B_0) & 0 \\ 0 & P_{ac}(B_0) \end{pmatrix} \equiv \tilde{P}_{ac}(B_0)$$

Now, for $\varphi \in \mathscr{H}_0$,

$$\begin{aligned} W_1(-t)JW_0(t)P_{ac}(A_0)\varphi &= T_1^{-1}\tilde{W}_1(-t)T_1 J T_0^{-1}\tilde{W}_0(t)T_0 P_{ac}(A_0)\varphi \\ &= T_1^{-1}\tilde{W}_1(-t)\tilde{V}\tilde{W}_0(t)\tilde{P}_{ac}(B_0)\varphi \\ &= (T_1^{-1}\tilde{V})(\tilde{V}^{-1}\tilde{W}_1(-t)\tilde{V})\tilde{W}_0(t)\tilde{P}_{ac}(B_0)\varphi \end{aligned}$$

Since

$$\tilde{V}^{-1}\tilde{W}_1(-t)\tilde{V} = \begin{pmatrix} e^{iV^{-1}B_1Vt} & 0 \\ 0 & e^{-iV^{-1}B_1Vt} \end{pmatrix}$$

we have

$$(\tilde{V}^{-1}\tilde{W}_1(-t)\tilde{V})\tilde{W}_0(t) = \begin{pmatrix} e^{iV^{-1}B_1Vt}e^{-iB_0t} & 0 \\ 0 & e^{-iV^{-1}B_1Vt}e^{iB_0t} \end{pmatrix}$$

Therefore $\lim_{t\to\pm\infty} W_1(-t)JW_0(t)P_{ac}(A_0)\varphi$ will exist for all $\varphi \in \mathscr{H}_0$ if and only if $\lim_{t\to\pm\infty} e^{iV^{-1}B_1Vt}e^{-iB_0t}P_{ac}(B_0)\psi$ exist for all $\psi \in \mathscr{K}_0$.

Since J is unitary, it is invertible. J^{-1} is automatically an A_0 left inverse of J and J is a A_1 left inverse of J^{-1}. Thus, according to Proposition 5c in Section 3, to show that $\Omega^{\pm}(A_1, A_0; J)$ are complete we need only show that $\Omega^{\pm}(A_0, A_1, J^{-1})$ exist. By a similar argument to the above, this is equivalent to the existence of the limits s-$\lim_{t\to\pm\infty} e^{iB_0t}e^{-iV^{-1}B_1Vt}P_{ac}(V^{-1}B_1V)$, which is equivalent to the completeness of $\Omega^{\pm}(V^{-1}B_1V, B_0)$ according to Proposition 3 of Section 3. ∎

It is clear from the above argument why J is such a convenient identification operator. However, from a physical point of view, J is artificial. For example, suppose that $\mathscr{K}_0$ and $\mathscr{K}_1$ are setwise equal with equivalent inner products, that the quadratic form domains of H_0 and H_1 are equal, and that

$$d_0(u, H_0u)_{\mathscr{K}_0} \le (u, H_1u)_{\mathscr{K}_1} \le d_1(u, H_0u)_{\mathscr{K}_0} \tag{193}$$

Equivalently,

$$d_0\|B_0u\|^2_{\mathscr{K}_0} \le \|B_1u\|^2_{\mathscr{K}_1} \le d_1\|B_0u\|^2_{\mathscr{K}_0}$$

so $\mathscr{H}_0$ and $\mathscr{H}_1$ are setwise equal with equivalent inner products. In this situation (which holds in the example of acoustic scattering), it is natural to use the identity $I_{01}: \mathscr{H}_0 \to \mathscr{H}_1$ as identification operator, and to ask about the existence and completeness of $\Omega^{\pm}(A_1, A_0, I_{01})$. We use the pedantic symbol I_{01} because we shall later consider I_{01}^* which is not equal to I_{10}. Suppose that a unitary $V: \mathscr{K}_0 \to \mathscr{K}_1$ is given and that we know from Theorem XI.75 that $\Omega^{\pm}(A_1, A_0; J)$ exist. If J and I_{01} are asymptotically A_0-equivalent, that is, if

$$\lim_{t\to\pm\infty} (J - I_{01})W_0(t)P^0_{ac}(A_0)\varphi = 0 \tag{194}$$

for all $\varphi \in \mathscr{H}_0$, then according to Proposition 5a of Section 3, $\Omega^{\pm}(A_1, A_0; I_{01})$ exist and equal $\Omega^{\pm}(A_1, A_0, J)$. Since $J\langle u, v\rangle = \langle B_1^{-1}VB_0u, Vv\rangle$, we expect (194) to hold only if V behaves B_0-asymptotically like the identity operator and B_0 and B_1 are asymptotically equal. Technically, we formulate the second condition by requiring that

$$\|(H_0 - V^{-1}H_1V)e^{-iB_0t}w\|_{\mathscr{K}_0} \to 0 \quad \text{as} \quad t \to \pm\infty \tag{195}$$

for all w in a dense set $\mathscr{D} \subset D(H_0) \cap D(V^{-1}H_1V) \cap P_{ac}(H_0)$ that is invariant under e^{itB_0}, B_0, and B_0^{-1}. The first condition is met by requiring that

$$\|(I + V^{-1}H_1V)(V^{-1} - I)e^{-iB_0t}w\|_{\mathscr{K}_0} \to 0 \quad \text{as} \quad t \to \pm\infty \tag{196}$$

for all $w \in \mathscr{D}$.

Theorem XI.76 Let $\mathscr{K}_k$, $\mathscr{H}_k$, H_k, B_k, A_k, $k = 0, 1$, V, J, and I_{01} be as defined above. Suppose that:

(i) $\mathscr{K}_0$ and $\mathscr{K}_1$ are setwise equal with equivalent inner products.
(ii) $Q(H_0) = Q(H_1)$ setwise and that (193) holds.
(iii) (195) and (196) hold.
(iv) The wave operators $\Omega^{\pm}(V^{-1}B_1V, B_0)$ exist on $\mathscr{K}_0$.

Then (194) holds, so, in particular, $\Omega^{\pm}(A_1, A_0; I_{01})$ exist and equal $\Omega^{\pm}(A_1, A_0; J)$.

Proof Let w_0 and w_1 be in $\mathscr{D}$ and set $\varphi = \langle w_0, w_1\rangle$. Since $\mathscr{D}$ is dense in $P_{ac}(H_0)$ and $(I_{01} - J)W_0(t)$ are uniformly bounded, it is sufficient to prove (194) for such φ. Let $u_0(t)$ and $v_0(t)$ be the components of $W_0(t)\varphi$. Then, since $\varphi \in P_{ac}(A_0)$, we have

$$\begin{aligned} &\|(J - I_{01})W_0(t)P_{ac}(A_0)\varphi\|^2_{\mathscr{H}_1} \\ &\quad = \|B_1(B_1^{-1}VB_0 - I)u_0(t)\|^2_{\mathscr{K}_1} + \|(V - I)v_0(t)\|^2_{\mathscr{K}_1} \\ &\quad = \|(B_0 - V^{-1}B_1)u_0(t)\|^2_{\mathscr{K}_0} + \|(I - V^{-1})v_0(t)\|^2_{\mathscr{K}_0} \end{aligned}$$

Since $v_0(t) = -B_0(\sin B_0 t)w_0 + (\cos B_0 t)w_1$ and $w_k \in \mathscr{D}$, (196) and the positivity of H_1 imply that the second term goes to zero as $t \to \pm\infty$. We estimate the first term by

$$\|(B_0 - V^{-1}B_1)u_0(t)\|_{\mathscr{H}_0}$$
$$\leq \|(B_0 - V^{-1}B_1 V)u_0(t)\|_{\mathscr{H}_0} + \|(V^{-1}B_1 V)(I - V^{-1})u_0(t)\|_{\mathscr{H}_0}$$

As above, the second term goes to zero by (196). For notational simplicity, set $B_1' = V^{-1}B_1 V$ and denote $\Omega^{\pm}(B_1', B_0)$ simply by $\Omega^{\pm}$. We must show that

$$\|(B_0 - B_1')e^{-itB_0}w\|_{\mathscr{H}_0} \to 0 \qquad \text{as} \quad t \to \pm\infty$$

or equivalently

$$\|e^{itB_1'}(B_0 - B_1')e^{-itB_0}w\|_{\mathscr{H}_0} \to 0 \qquad \text{as} \quad t \to \pm\infty$$

for w in $\mathscr{D}$. By (iv),

$$e^{iB_1't}B_0 e^{-iB_0t}w \to \Omega^+ B_0 w \qquad \text{as} \quad t \to -\infty$$

Thus, to conclude the result in the case $t \to -\infty$, it is sufficient to show that

$$e^{iB_1't}B_1' e^{-iB_0t}w = B_1' e^{iB_1't}e^{-iB_0t}w \to B_1'\Omega^+ w$$

since $B_1'\Omega_+ w = \Omega_+ B_0 w$. If we take $w \in \mathscr{D}$ and expand

$$\|B_1' e^{iB_1't}e^{-iB_0t}w - B_1'\Omega^+ w\|_{\mathscr{H}_0}^2 = \|B_1' e^{iB_1't}e^{-iB_0t}w\|_{\mathscr{H}_0}^2 + \|B_1'\Omega^+ w\|_{\mathscr{H}_0}^2$$
$$- (B_1' e^{iB_1't}e^{-iB_0t}w, B_1'\Omega^+ w)_{\mathscr{H}_0}$$
$$- (B_1'\Omega^+ w, B_1' e^{iB_1't}e^{-iB_0t}w)_{\mathscr{H}_0}$$

we see that, by taking B_1' to the other side, the last two terms converge to $-\|B_1'\Omega_+ w\|_{\mathscr{H}_0}^2$. Thus, to show that the whole expression goes to zero we need just prove that

$$\lim_{t\to-\infty} \|B_1' e^{iB_1't}e^{-iB_0t}w\|_{\mathscr{H}_0}^2 \leq \|B_1'\Omega^+ w\|_{\mathscr{H}_0}^2$$

We compute,

$$\begin{aligned}
\overline{\lim_{t\to-\infty}} \|B_1' e^{iB_1't}e^{-iB_0t}w\|_{\mathscr{H}_0}^2 &= \overline{\lim_{t\to-\infty}} (e^{-iB_0t}w, H_1' e^{-iB_0t}w)_{\mathscr{H}_0} \\
&= \overline{\lim_{t\to-\infty}} (e^{-iB_0t}w, H_0 e^{-iB_0t}w)_{\mathscr{H}_0} \\
&= \|B_0 w\|_{\mathscr{H}_0}^2 \\
&= \|\Omega_+ B_0 w\|_{\mathscr{H}_0}^2 \\
&= \|B_1'\Omega_+ w\|_{\mathscr{H}_0}^2 \qquad (197)
\end{aligned}$$

In the second step we used (195). This proves (194) in the case $t \to -\infty$. The other case is similar. ∎

Notice that all the hypotheses in Theorems XI.75 and XI.76 deal with H_0 and $H_1' = V^{-1}H_1 V$ on $\mathscr{H}_0$. Thus the two Hilbert space scattering problem on $\mathscr{H}_0$ and $\mathscr{H}_1$ is reduced to studying the scattering theory for two self-adjoint operators on a single Hilbert space $\mathscr{H}_0$. In fact, if we changed our point of view slightly, we could reformulate Theorems XI.75 and XI.76 to avoid the two Hilbert space scattering theory entirely. For, if hypotheses (i) and (ii) of Theorem XI.76 hold, then $W_1(t)$ is a strongly continuous group of bounded operators on $\mathscr{H}_0$ (in general, not a unitary group). Hypotheses (iii) and (iv) give conditions on H_0 and $V^{-1}H_1 V$ on $\mathscr{H}_0$ so that the "wave operators"

$$\text{s-lim}_{t\to\mp\infty} W_1(-t)W_0(t)P_{\text{ac}}(A_0)$$

exist on $\mathscr{H}_0$. And, according to Theorem XI.75, if $\Omega^{\pm}(V^{-1}H_1 V, H_0)$ are complete, then these wave operators are complete as maps from $\mathscr{H}_0$ to $\mathscr{H}_0$.

Example 1, continued We can now apply these theorems to acoustic scattering. In addition to hypotheses (188) and (190) we assume that $c(x)$ and $\rho(x)$ are twice continuously differentiable with bounded derivatives. These smoothness assumptions can be avoided; see the discussion at the end of the section. We define $\mathscr{H}_0 = L^2(\mathbb{R}^3) = \mathscr{H}_1$ with inner products

$$(u, v)_{\mathscr{H}_0} = (c_0^2\rho_0)^{-1}(u, v)_{L^2(\mathbb{R}^3)}$$
$$(u, v)_{\mathscr{H}_1} = (u, (c(x)^2\rho(x))^{-1}v)_{L^2(\mathbb{R}^3)}$$

The operators H_k, B_k, and A_k are as described in Example 1. In particular, $D(B_0) = D(B_1)$ and (193) holds. Thus conditions (i) and (ii) of Theorem XI.76 hold, so the Hilbert spaces $\mathscr{H}_0$ and $\mathscr{H}_1$ constructed from $\mathscr{H}_0$ and $\mathscr{H}_1$ as above are setwise equal with equivalent inner products. We naturally choose V to be the unitary map $V: \mathscr{H}_0 \to \mathscr{H}_1$ given by

$$V: u(x) \mapsto [c(x)^2\rho(x)/c_0^2\rho_0]^{1/2}u(x)$$

so

$$V^{-1}H_1 V = -[c(x)^2\rho(x)]^{1/2}(\nabla \cdot \rho(x)^{-1}\nabla)[c(x)^2\rho(x)]^{1/2}$$

To verify (195) and (196), we choose $\mathscr{D}$ to be the set of $f \in \mathscr{S}(\mathbb{R}^3)$ whose Fourier transforms have support away from the origin. Notice that $(H_0 - V^{-1}H_1 V)e^{-iB_0t}w$ and $(I + V^{-1}H_1 V)(V^{-1} - I)e^{-iB_0t}w$ can both be written as sums of terms of the form

$$f(x)e^{\pm iB_0t}P(D)w$$

where $P(D)$ is a constant coefficient partial differential operator and $f(x)$ is a product of terms of the form $\rho(x) - \rho_0$, $c(x) - c_0$, $\rho(x)$, ρ_0, $c(x)$, c_0, or their inverses or square roots, or their derivatives up to order two. Moreover, at least one factor of $\rho(x) - \rho_0$, $c(x) - c_0$, $D^\alpha\rho(x)$, or $D^\alpha c(x)$, $0 \neq |\alpha| \leq 2$, occurs. For $w \in \mathscr{D}$, $e^{\pm iB_0 t}P(D)w$ is a regular wave packet for the free wave equation ($m = 0$) in three dimensions, so by Theorem XI.18,

$$\|e^{\pm iB_0 t}P(D)w\|_\infty \leq c/|t|$$

Thus, if we require that $\rho(x) - \rho_0, c(x) - c_0, D^\alpha\rho(x), D^\alpha c(x), 0 \neq |\alpha| \leq 2$, be in $L^2(\mathbb{R}^3)$, then

$$\|f(x)e^{\pm iB_0 t}P(D)w\|_{\mathscr{H}_0} \to 0 \qquad \text{as} \quad t \to \pm\infty$$

for each of the terms, so (195) and (196) hold. An alternative proof which avoids stationary phase ideas is as follows: Since $\hat{w}$ has compact support, $E_{[-M,M]}(-\Delta)w = w$ for some M. Thus if $\rho(x) - \rho_0$, etc. are in $L^2_\delta(\mathbb{R}^3)$ for some $\delta > \frac{3}{2}$, then $f(x)E_{[-M,M]}(-\Delta)$ is Hilbert–Schmidt and thus compact. The convergence to zero then follows from Lemma 2 in Section 3.

It remains to investigate when $\Omega^\pm(V^{-1}B_1V, B_0)$ exist and are complete. We first apply Theorem XI.10 (Birman's theorem) to $V^{-1}H_1V$ and H_0. We already know that $D(B_1) = D(B_0)$, and, by the hypotheses on $\rho(x)$ and $c(x)$, $Q(H_0) = Q(V^{-1}H_0V)$. Thus $D(V^{-1}B_1V) = D(B_0)$, so $V^{-1}H_1V$ and H_0 are mutually subordinate. Furthermore,

$$H_0 - V^{-1}H_1V = (c(x)^2 - c_0^2)\Delta + h(x)\cdot\nabla + e(x)$$

where $h(x)$ and $e(x)$ are sums of functions of the form of $f(x)$ described above. Thus for each bounded interval I,

$$(H_0 - V^{-1}H_1V)E_I(H_0)$$

is a sum of operators of the form

$$f(x)g(-i\nabla)$$

where g is the product of a polynomial and the characteristic function of a finite interval. According to Theorem XI.21, $f(x)g(-i\nabla)$ will be trace class if $f \in L^2_\delta(\mathbb{R}^3)$ for some $\delta > \frac{3}{2}$. And, if $(H_0 - V^{-1}H_1V)E_I(H_0)$ is trace class, then $E_I(V^{-1}H_1V)(H_0 - V^{-1}H_1V)E_I(H_0)$ is automatically trace class since $E_I(V^{-1}H_1V)$ is bounded, so the conditions of Birman's theorem are fulfilled.

We have shown that if $c(x)^2 - c_0^2, \rho(x) - \rho_0, D^\alpha\rho(x), D^\alpha c(x), 0 \neq |\alpha| \leq 2$, are in $L^2_\delta(\mathbb{R}^3)$ for some $\delta > \frac{3}{2}$, then $\Omega^\pm(V^{-1}H_1V, H_0)$ exist and are complete. Since $\sqrt{x}$ is an admissible function, the invariance principle (Theorem XI.11) implies that $\Omega^\pm(V^{-1}B_1V, B_0)$ exist and are complete. Thus, applying Theorems XI.75 and XI.76 we have:

Theorem XI.77 Suppose that $c(x)$ and $\rho(x)$ are twice continuously differentiable functions with bounded derivatives satisfying (188) and (190). Suppose that $c(x)^2 - c_0^2$, $\rho(x) - \rho_0$, $D^\alpha\rho(x)$, $D^\alpha c(x)$, $0 \neq |\alpha| \leq 2$, are all in $L^2_\delta(\mathbb{R}^3)$ for some $\delta > \frac{3}{2}$. Then, the wave operators $\Omega^\pm(A_1, A_0; I_{01})$ associated with the systems (186), (187) exist and are complete.

We have proven completeness in the sense of generalized wave operators. It can be proven that $\mathscr{H}_{ac}(A_1) = \mathscr{H}_1$, so *every* solution of (187) is asymptotic to a free solution. We have essentially proven that A_1 has no singular continuous spectrum in the appendix to Section 6. We shall prove that A_1 has no eigenvalues in Section XIII.13.

The decay conditions on $c(x)^2 - c_0^2$, $\rho(x) - \rho_0$, $D^\alpha\rho(x)$, $D^\alpha c(x)$ are not very stringent in that they will hold in any reasonable physical situation. On the other hand, the smoothness hypotheses restrict the applicability of the theorem greatly since in many inhomogeneous media problems there is a sudden change in $\rho(x)$ or $c(x)$ as one passes from one medium to the next. Fortunately, the smoothness hypotheses can be removed.

Example 1, revisited Existence and completeness of the wave operators for acoustical scattering in an inhomogeneous medium can also be proven by applying the Birman–Belopol'skii theorem (Theorem XI.13) directly. We take $\mathscr{K}_k$, $\mathscr{H}_k$, A_k, H_k, and B_k to be as above and choose I_{01} as the identification operator from $\mathscr{H}_0$ to $\mathscr{H}_1$. We must verify that hypotheses (a)–(d) of Theorem XI.13 hold. (a) is obvious. Since $D(A_k) = D(B_k^2) \oplus D(B_k)$ and we already know that $D(B_0) = D(B_1)$, we need only prove that $D(H_0) = D(H_1)$ to conclude that (d_1) holds. And, since V takes $D(H_0)$ into itself, we need only prove that $V^{-1}H_1V$ and H_0 have the same domain on $\mathscr{K}_0$. The proof, which uses the symmetric form of the Kato–Rellich theorem (see Problem 66), is left to the reader.

To prove condition (b), we want to show that $(A_1 - A_0)E_I(A_0)$ is trace class as an operator from $\mathscr{H}_0$ to $\mathscr{H}_1$. Since the identity is bounded from $\mathscr{H}_0$ to $\mathscr{H}_1$, it is sufficient to show that $(A_1 - A_0)E_I(A_0)$ is trace class as an operator on $\mathscr{H}_0$. Set $C = B_0^2 - B_1^2$ and let T_0 be the unitary map $T_0: \mathscr{H}_0 \to \mathscr{K}_0 \oplus \mathscr{K}_0$ introduced in the proof of Theorem XI.75. Then

$$T_0(A_1 - A_0)E_I(A_0)T_0^{-1} = \frac{1}{2}\begin{pmatrix} -CB_0^{-1} & -CB_0^{-1} \\ CB_0^{-1} & CB_0^{-1}\end{pmatrix}\begin{pmatrix} E_I(B_0) & 0 \\ 0 & E_I(B_0)\end{pmatrix}$$

on $\mathscr{K}_0 \oplus \mathscr{K}_0 = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$. Since ∇B_0^{-1} is a bounded operator commuting with $E_I(B_0)$, the same proof as in Example 1 (continued) shows that $\pm CB_0^{-1}E_I(B_0)$ is trace class on $L^2(\mathbb{R}^3)$ if the conditions on $c(x)$ and $\rho(x)$

expressed in Theorem XI.77 hold. Therefore (b) holds under these conditions.

Finally, we must check (c). An easy calculation shows that $I_{01}^*: \mathscr{H}_1 \to \mathscr{H}_0$ is given by

$$I_{01}^* \langle u, v \rangle = \langle -(c_0^2 \rho_0) B_0^{-2} \nabla \cdot \rho(x)^{-1} \nabla u, (c_0^2 \rho_0 / c(x)^2 \rho(x)) v \rangle$$

Thus, we may write

$$(I_{01}^* I_{01} - I_{00}) \langle u, v \rangle = \langle Q_1 u, Q_2 v \rangle$$

where

$$Q_1 = -(c_0^2 \rho_0) B_0^{-2} \nabla \cdot (1/\rho(x)) \nabla - I$$
$$Q_2 = (c_0^2 \rho_0 / c(x)^2 \rho(x)) - I$$

Using the diagonalizing transformation T_0 as above, we find that

$$T_0 (I_{01}^* I_{01} - I_{00}) E_I(A_0) T_0^{-1}$$
$$= \frac{1}{2} \begin{pmatrix} B_0 Q_1 B_0^{-1} + Q_2 & B_0 Q_1 B_0^{-1} - Q_2 \\ B_0 Q_1 B_0^{-1} - Q_2 & B_0 Q_1 B_0^{-1} + Q_2 \end{pmatrix} \begin{pmatrix} E_I(B_0) & 0 \\ 0 & E_I(B_0) \end{pmatrix}$$

Thus, we are reduced to showing that $B_0 Q_1 B_0^{-1} E_I(B_0)$ and $Q_2 E_I(B_0)$ are compact as operators on $L^2(\mathbb{R}^3)$. For the second operator, this follows immediately if $c(x)$ and $\rho(x)$ obey the conditions of Theorem XI.77. For the first operator, notice that

$$B_0 Q_1 B_0^{-1} E_I(B_0) = -(c_0^2 \rho_0)(B_0^{-1} \nabla) \cdot \left(\frac{1}{\rho(x)} - \frac{1}{\rho_0} \right) (\nabla B_0^{-1}) E_I(B_0)$$

Since $B_0^{-1} \nabla$ is bounded and $(\rho(x)^{-1} - \rho_0^{-1})(\nabla B_0^{-1}) E_I(B_0)$ is trace class by Theorem XI.21, $B_0 Q_1 B_0^{-1} E_I(B_0)$ is trace class and therefore compact. We conclude that $(I_{01}^* I_{01} - I_{00}) E_I(A_0)$ is compact if $\rho(x)$ satisfies the conditions of Theorem XI.77.

We have verified conditions (a)–(d_1) of the Birman–Belopol'skii theorem, so the wave operators $\Omega^{\pm}(A_1, A_0; I)$ exist and are complete. Notice that using the Birman–Belopol'skii theorem does not avoid completely the reduction to a single Hilbert space since we must make the reduction to verify the hypotheses. The reason that we have avoided explicit proof of (195) and (196) is that we have used a compactness argument, as we could have in the verification of (195) and (196).

Example 2 (optical scattering) The scattering of electromagnetic waves in an inhomogeneous medium is governed by Maxwell's equations:

$$\nabla \times E = -\mu(x) \frac{\partial H}{\partial t} \qquad \nabla \times H = \varepsilon(x) \frac{\partial E}{\partial t}$$
$$\nabla \cdot (\varepsilon(x) E) = 0 \qquad \nabla \cdot (\mu(x) H) = 0 \tag{198}$$

E and H are functions from $\mathbb{R}^3$ to $\mathbb{R}^3$ representing the electric and magnetic fields. $\varepsilon(x)$ and $\mu(x)$ are three-by-three matrix-valued functions on $\mathbb{R}^3$ representing the dielectric and magnetic susceptibilities. We assume that $\varepsilon(x)$ and $\mu(x)$ are C^2 with bounded derivatives; and since we want the energy

$$(E, H) = \int_{\mathbb{R}^3} [\overline{E(x)} \cdot \varepsilon(x) E(x) + \overline{H(x)} \cdot \mu(x) H(x)] \, dx$$

to be positive, we require that

$$c_1 I \leq \varepsilon(x) \leq c_2 I, \qquad c_3 I \leq \mu(x) \leq c_4 I \tag{199}$$

for all x for some positive constants c_i. Suppose that there are constant positive definite matrices ε_0 and μ_0 so that

$$\varepsilon(x) \to \varepsilon_0, \qquad \mu(x) \to \mu_0$$

as $|x| \to \infty$. Then we should be able to develop a scattering theory for (198) in terms of the free equations

$$\nabla \times E = -\mu_0 \frac{\partial H}{\partial t} \qquad \nabla \times H = \varepsilon_0 \frac{\partial E}{\partial t}$$
$$\nabla \cdot (\varepsilon_0 E) = 0 \qquad \nabla \cdot (\mu_0 H) = 0 \tag{200}$$

In order to do this we rewrite (198) as a second-order equation for E:

$$\ddot{E} = -\varepsilon^{-1} \nabla \times (\mu^{-1} (\nabla \times E)) \tag{201}$$

and similarly for (200). Now, define $\mathscr{H}_0$ and $\mathscr{H}_1$ to be $L^2(\mathbb{R}^3)^3$ with inner products

$$(E, F)_{\mathscr{H}_0} \equiv \int_{\mathbb{R}^3} \overline{E(x)} \cdot \varepsilon_0 F(x) \, dx$$

$$(E, F)_{\mathscr{H}_1} \equiv \int_{\mathbb{R}^3} \overline{E(x)} \cdot \varepsilon(x) F(x) \, dx$$

Let $\mathcal{Q} = \{E \in L^2(\mathbb{R}^3)^3 \,|\, \nabla \times E \in (L^2)^3\}$ and define quadratic forms q_0 and q_1 on $\mathcal{Q}$ by

$$q_0(E, F) = \int_{\mathbb{R}^3} (\nabla \times E) \cdot \mu_0^{-1}(\nabla \times F)\, dx$$

$$q_1(E, F) = \int_{\mathbb{R}^3} (\nabla \times E) \cdot \mu(x)^{-1}(\nabla \times F)\, dx$$

q_0 and q_1 are the quadratic forms of positive self-adjoint operators on $\mathscr{K}_0$ and $\mathscr{K}_1$, respectively,

$$H_0 E = -\varepsilon_0^{-1} \nabla \times \mu_0^{-1}(\nabla \times E)$$

$$H_1 E = -\varepsilon(x)^{-1} \nabla \times \mu(x)^{-1}(\nabla \times E)$$

and the square roots of these operators satisfy (193) because of (199). Finally, we define $V: \mathscr{K}_0 \to \mathscr{K}_1$ by

$$(VE)(x) = \varepsilon(x)^{-1/2} \varepsilon_0^{1/2} E(x)$$

We are thus in the situation covered by Theorems XI.75 and XI.76 except that H_0 and H_1 have point spectrum at zero. This does not cause any difficulty in these theorems for they can easily be extended to handle this case; see the reference in the Notes. Thus, as in Example 1, the scattering problem can be reduced to studying H_0 and $V^{-1} H_1 V$ on $\mathscr{K}_0$. (195) and (196) follow as in Example 1 since $P_{ac}(H_0)$ projects out the zero modes and each component of $e^{\pm iB_0 t} P_{ac}(B_0) w$ obeys a free wave equation and thus satisfies

$$\| e^{\pm iB_0 t} P_{ac}(B_0) w \|_\infty < c/t$$

Using this estimate, stationary phase, and Cook's method, one can easily show that the wave operators $\Omega^\pm(V^{-1} H_1 V, H_0)$ exist. Thus one obtains the existence of $\Omega^\pm(A_1, A_0; I_{01})$ analogously to Example 1.

The zero modes do cause a new difficulty in the proof of completeness, however, since one can no longer expect

$$(V^{-1} H_1 V - H_0) E_I(H_0)$$

to be trace class when the interval I contains zero. One possible way out would be to try to prove the existence of the limits

$$e^{iH_0 t} e^{-iV^{-1} H_1 V t} P_{ac}(V^{-1} H_1 V) w$$

directly by using Cook's method. But this is very difficult since

$$e^{-iV^{-1} H_1 V t} P_{ac}(V^{-1} H_1 V) w$$

will satisfy a wave equation with nonconstant coefficients and thus one cannot use the Fourier transform to prove estimates. Instead, one gets around the difficulty as follows. Define operators $\tilde{H}_k$ on $\mathscr{K}_k$ by the quadratic forms

$$\tilde{q}_k(E, F) = q_k(E, F) + \int (\nabla \cdot \gamma_k E) \cdot (\nabla \cdot \gamma_k F)\, dx$$

where $\gamma_0 = \varepsilon_0$ and $\gamma_1 = \varepsilon(x)$. One can prove that

$$(V^{-1} \tilde{H}_1 V + 1)^{-2} - (\tilde{H}_0 + 1)^{-2}$$

is trace class, essentially because the addition of the extra term has removed the zero modes and made $V^{-1} \tilde{H}_1 V$ and $\tilde{H}_0$ strictly elliptic. The existence and completeness of $\Omega^\pm(V^{-1} \tilde{H}_1 V, \tilde{H}_0)$ then follows from Corollary 2 of Theorem XI.11. Finally, one shows by an elementary argument that the existence of $\Omega^\pm(\tilde{H}_0, V^{-1} \tilde{H}_1 V)$ implies the existence of $\Omega^\pm(H_0, V^{-1} H_1 V)$. The reason is that the dynamical modes and the zero modes are completely decoupled in Maxwell's equations, so giving a spurious dynamics to the zero modes does not affect the dynamical modes. For details, see the reference in the Notes.

Example 3 (scattering of acoustical waves from obstacles) Let $\mathcal{O}$ be a closed bounded set in $\mathbb{R}^3$ whose boundary Γ has measure zero and whose complement is connected. Then the acoustic wave equation in the exterior of the obstacle $\mathcal{O}$ is

$$\begin{aligned} u_{tt} - \Delta u &= 0, && x \in \mathbb{R}^3 \backslash \mathcal{O} \\ \frac{\partial u}{\partial \hat{n}} &= 0, && x \in \Gamma \\ u(x, 0) &= f(x), && x \in \mathbb{R}^3 \backslash \mathcal{O} \\ u_t(x, 0) &= g(x), && x \in \mathbb{R}^3 \backslash \mathcal{O} \end{aligned} \tag{202}$$

where u is the difference between the pressure at x at time t and the equilibrium pressure. The Neumann boundary conditions can be understood as follows: A pressure gradient causes a proportional fluid flow. Thus the condition $\nabla u \cdot \hat{n} = 0$ on Γ just says that there is no flow across Γ. Given an initial disturbance $\langle f(x), g(x) \rangle$ exterior to the obstacle, the solution of (202) will depend on the geometry of the obstacle; but for large positive and negative times, the waves should propagate away from the obstacle to infinity. As more and more of the energy goes away from the obstacle, the solution of (202) should look more and more like a solution of $u_{tt} - \Delta u = 0$

on all of $\mathbb{R}^3$. Thus, we expect to be able to construct a scattering theory for (202) in terms of the solutions of the free wave equation.

We can choose the same Hilbert space for H_0 and H_1 by the simple expedient of allowing the interior of the obstacle to have acoustic disturbances. Since the interior and the exterior are decoupled, this does not affect the scattering theory. Let H_0 denote $-\Delta$ on $L^2(\mathbb{R}^3)$ and let H_1 be the Neumann Laplacian H_N on $L^2(\mathbb{R}^3)$ with boundary Γ as defined in Section XIII.15. Thus in this case, we have $\mathscr{H}_0 = L^2(\mathbb{R}^3) = \mathscr{H}_1$ and because of the boundary conditions, $Q(H_N) \supset Q(H_0)$. Further, for $w \in Q(H_0)$, we have

$$\|B_0 w\|_2^2 = \|B_N w\|_2^2 \tag{203}$$

The only difficulty applying the abstract theory developed in Theorem XI.75 is that if Γ separates $\mathbb{R}^3$ into more than one connected component, then B_1 will have zero as an eigenvalue: $H_N \varphi = 0$ and $\varphi \in L^2(\mathbb{R}^3)$ if φ is constant on one of the bounded connected components. Physically, these eigenfunctions are irrelevant to the problem since they are *interior* to the obstacle. Mathematically, one can overcome this difficulty by extending Theorem XI.75 so that it allows point spectrum at zero (see the reference in the Notes) or by the following simple expedient: We redefine H_N on each such internal constant eigenfunction φ so that $H_N \varphi = \varphi$. Assuming that there are only finitely many connected internal components, this redefinition does not affect any of the trace class conditions mentioned below or proven in the appendix. Having redefined H_N in this way we can apply the theory developed in this section. In particular, by Theorem XI.75, $\Omega^{\pm}(A_N, A_0; J)$ exist and are complete from $\mathscr{H}_0$ to $\mathscr{H}_1$ if $\Omega^{\pm}(H_N, H_0)$ exist and are complete on $\mathscr{H}_0 = L^2(\mathbb{R}^3)$. Here J: $\langle u, v\rangle \mapsto \langle B_N^{-1} B_0 u, v\rangle$. In the appendix we show how to prove that $(H_N + 1)^{-2} - (H_0 + 1)^{-2}$ is trace class and thus, by Corollary 3 of Theorem XI.11, $\Omega^{\pm}(H_N, H_0)$ exist and are complete.

It is no longer true that $\mathscr{H}_0 = \mathscr{H}_1$ since (193) does not hold in this case. However, since $Q(H_0) \subset Q(H_N)$ and (203) holds, $\mathscr{H}_0$ can be naturally imbedded as a subspace of $\mathscr{H}_1$. Therefore, it is natural to choose this embedding as the identification operator. Notice that (193) is not used anywhere in the proof of Theorem XI.76 although it is needed to have $\mathscr{H}_0 = \mathscr{H}_1$. Since $V = I$, condition (196) holds automatically; and because of (203), condition (195) is not necessary. For the proof of Theorem XI.76 goes through as before except that the crucial equality (197) holds because of (203) without appealing to (193) and (195). Thus $\Omega^{\pm}(A_N, A_0; I)$ exist and are complete.

The case of scattering from an obstacle with Dirichlet boundary conditions is less interesting physically; but because the corresponding local compactness result is simpler (see the appendix), it is a good test case for various

approaches to scattering theory. Let $H_1 = H_D$, the Dirichlet Laplacian with boundary Γ as defined in Section XIII.15. Then $Q(H_D) \subset Q(H_0)$ and

$$\|B_0 w\|_2^2 = \|B_D w\|_2^2 \tag{204}$$

for $w \in Q(H_D)$. Thus we have a similar setup to the one above except that $Q(H_D) \subset Q(H_0)$, whereas in the Neumann case $Q(H_N) \supset Q(H_0)$. Therefore we deal with the adjoints of the usual wave operators. Theorem XI.75 shows that $\Omega^{\pm}(A_0, A_D, J')$ exist and are complete as maps from $\mathscr{H}_1$ to $\mathscr{H}_0$ if $\Omega^{\pm}(H_0, H_D)$ exist and are complete on $\mathscr{H}_1 = L^2(\mathbb{R}^3)$. Here J': $\langle u, v\rangle \mapsto \langle B_0^{-1} B_D u, v\rangle$. In the appendix we show that $(H_0 + 1)^{-2} - (H_D + 1)^{-2}$ is trace class so, as above, the existence and completeness of $\Omega^{\pm}(H_0, H_D)$ follow from Corollary 3 of Theorem XI.11. By the same idea described above, the conclusions of Theorem XI.76 follow automatically from (204), so J' may be replaced by the embedding I_{10} taking $\mathscr{H}_1$ into $\mathscr{H}_0$. That is, $\Omega^{\pm}(A_0, A_D; I_{10})$ exist and are complete. Since I_{10} is an isometry, I_{10}^* is an A_D-left inverse for I_{10}. Thus, by Proposition 5c of Section 3, $\Omega^{\pm}(A_D, A_0; I_{10}^*)$ exist and are complete.

We have proven:

Theorem XI.78 Let $\mathcal{O}$ be a closed bounded set in $\mathbb{R}^3$ with boundary Γ.

(a) If Γ has measure zero, if $\mathbb{R}^3 \backslash \Gamma$ has finitely many connected components, and if Γ obeys the regularity condition of Theorem XI.81, then the wave operators for the equation (202) with Neumann boundary conditions exist and are complete.

(b) If Γ has measure zero, then the wave operators for (202) with Dirichlet boundary conditions exist and are complete.

In Examples 1 and 2 we assumed that the coefficients describing the inhomogeneity were C^2 functions of the space variables. This is a very restrictive condition since some of the most interesting physical problems involve sharp changes in wave velocities or densities when passing from one medium to another. Fortunately, one can handle the nonsmooth case without great difficulty. Notice that in Example 1 we did not use any smoothness of $\rho(x)$ in defining H_1 on $\mathscr{H}_1$ and, of course, no smoothness is used in the abstract theorems. The only place that we used smoothness was in verifying that $(V^{-1} H_1 V - H_0) E_I(H_0)$ is trace class on $L^2(\mathbb{R}^3)$; we needed to express $V^{-1} H_1 V - H_0$ as a sum of terms of the form $f(x)P(D)$, so we could apply Theorem XI.21. P. Deift has shown how to use the commutation formula

$$\frac{\lambda}{BA + \lambda} + B \frac{1}{AB + \lambda} A = 1 \tag{205}$$

to avoid this difficulty. If A and B are bounded operators on a Hilbert space $\mathscr{H}$, then $\sigma(AB)\backslash\{0\} = \sigma(BA)\backslash\{0\}$ and for $-\lambda \notin \sigma(AB) \cup \{0\}$, (205) holds. The reader is asked to provide a proof in Problem 115. More generally, if A is a closed operator and $B = A^*$, then (205) holds for $-\lambda \in \mathbb{C}\backslash[0, \infty)$. To see how to use (205), consider the one-dimensional case where the notation is the simplest. Then $H_1' = V^{-1}H_1 V = -aDb^2Da$ and $H_0 = D^2$ where $D = i\, d/dx$ and a and b are functions of x satisfying

$$0 < a_0 \leq a(x) \leq a_1, \qquad 0 \leq b_0 \leq b(x) \leq b_1$$

and we assume that $a(x) \to 1$, $b(x) \to 1$ sufficiently fast as $|x| \to \infty$. As in Example 1, we define H_1' as follows: Let Db^2D be the self-adjoint operator on $L^2(\mathbb{R})$ corresponding to the closure of the symmetric quadratic form $q(\varphi, \varphi) = (D\varphi, b^2D\varphi)_{L^2}$ on $C_0^\infty(\mathbb{R}) \times C_0^\infty(\mathbb{R})$. Since multiplication by a has a bounded inverse, $H_1' = aDb^2Da$ is a well-defined self-adjoint operator. We want to prove that

$$\frac{1}{aDb^2Da + 1} - \frac{1}{D^2 + 1}$$

is trace class. Using the formula

$$\frac{1}{aDb^2Da + 1} = a^{-1}\left(\frac{1}{Db^2D + a^{-2}}\right)a^{-1}$$

and the properties of a, this problem is easily reduced to proving that

$$\frac{1}{Db^2D + 1} - \frac{1}{D^2 + 1}$$

is trace class. Let A be the operator bD. Then since we defined Db^2D by using quadratic forms, $Db^2D = (bD)^*(bD)$ (see Section X.3) where bD denotes the operator closure of $bD \upharpoonright C_0^\infty(\mathbb{R})$. Setting $B = (bD)^*$ and applying the commutation formula, we have

$$\begin{aligned}\frac{1}{(bD)^*(bD) + 1} &= 1 - (bD)^*\left(\frac{1}{(bD)(bD)^* + 1}\right)(bD) \\ &= 1 - D^*\left(\frac{1}{D^*D + b^{-2}}\right)D\end{aligned}$$

and hence

$$\frac{1}{Db^2D + 1} - \frac{1}{D^2 + 1} = D^*\left(\frac{1}{D^*D + 1} - \frac{1}{D^*D + b^{-2}}\right)D$$

Thus, one is reduced to studying

$$\frac{1}{D^*D + 1} - \frac{1}{D^*D + 1 + (b^{-2} - 1)}$$

which can be handled by the usual methods for dealing with perturbations of $-d^2/dx^2$ by a potential. Essentially, the commutation formula allows us to unwrap Db^2D and get the b's on the outside.

The ideas in the three-dimensional case (discussed in the reference in the Notes) are the same with two exceptions. $D = i\nabla$ so bD is an operator from $L^2(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3)^3$ and $(bD)^*$ is an operator from $L^2(\mathbb{R}^3)^3$ to $L^2(\mathbb{R}^3)$. Thus one extends the commutation formula to the case where A is a closed operator from one Hilbert space to another and $B = A^*$. Also it is necessary to deal with the squares of the resolvents.

If the discontinuities of a and b lie in a compact set, one can also study the problem by using the twisting trick of the appendix to Section XI.11.

Appendix to XI.10: Trace class properties of Green's functions

Let Γ be a closed bounded subset of measure zero in $\mathbb{R}^n$. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$ and let $H_{\Gamma;D}$ and $H_{\Gamma;N}$ be $-\Delta$ on $L^2(\mathbb{R}^n)$ with Dirichlet and Neumann boundary conditions on Γ as defined in Section XIII.15. Set $R_0 = (H_0 + 1)^{-1}$, $R_{\Gamma;D} = (H_{\Gamma;D} + 1)^{-1}$, $R_{\Gamma;N} = (H_{\Gamma;N} + 1)^{-1}$. In this appendix we shall prove that $R_0^2 - R_{\Gamma;D}^2$ and $R_0^2 - R_{\Gamma;N}^2$ are trace class under suitable hypotheses on Γ when $n = 3$. Similar methods work for $n \neq 3$ if R^2 is replaced by R^m where $m > \frac{1}{2}n$ (Problem 116). Applications of these methods to the scattering of acoustical waves from obstacles appear in Example 3 of this section.

The basic results are:

Theorem XI.79 Let Γ be an arbitrary closed bounded subset of measure zero in $\mathbb{R}^3$. Then $R_0^2 - R_{\Gamma;D}^2$ is trace class.

Theorem XI.80 Let Γ be a closed bounded subset of measure zero in $\mathbb{R}^3$. Let B be an open ball containing Γ and let $\tilde{H}_{\partial B \cup \Gamma;N}$ be $-\Delta$ on $L^2(B)$ with Neumann boundary conditions on $\Gamma \cup \partial B$. Set

$$\tilde{R}_{\partial B \cup \Gamma;N} = (H_{\partial B \cup \Gamma;N} + 1)^{-1}$$

and suppose that $\tilde{R}_{\partial B \cup \Gamma;N}^2$ is trace class. Then $R_0^2 - R_{\Gamma;N}^2$ is trace class.

Notice that $R_0^2 - R_{\Gamma;D}^2 \in \mathscr{I}_1$ for any Γ, but we need restrictions on Γ in the Neumann case. The following example shows that these restrictions are necessary:

Example Let Λ be the union of an infinite number of disjoint balls of smaller and smaller radii all within the unit ball and let $\Gamma = \partial\Lambda$. Then $H_{\Gamma;N}$ has zero as an eigenvalue of infinite multiplicity and the corresponding eigenfunctions have support in the ball. If χ is multiplication by the characteristic function of the ball, then $\chi R_{\Gamma;N}^m$ is not compact for any m. On the other hand χR_0^m is compact for any $m \geq 2$ by Theorem XI.21, so $R_0^m - R_{\Gamma;N}^m$ is not compact for any m.

Of course, Theorem XI.80 is not very useful unless there are conditions that guarantee that $\tilde{R}_{\partial B \cup \Gamma;N}^2$ is trace class. In fact, there are very general sufficient conditions:

Definition A **truncated cone at** $x \in \mathbb{R}^n$ is a set of the form

$$\{y \mid 0 < |y - x| < \varepsilon, (y - x) \cdot n > (1 - \delta)|y - x|\}$$

for some $\varepsilon, \delta > 0$ and some unit vector n. An open set $\Lambda \subset \mathbb{R}^n$ with bounded boundary is said to have the **restricted cone property** if and only if there is a finite open cover $U_1, \ldots, U_k$ of $\partial\Lambda$ and truncated cones $C_1, \ldots, C_k$ at 0 so that $C_i + x \subset \Lambda$ if $x \in U_i \cap \Lambda$.

It is not hard to see that polyhedra and sets with smooth boundary have the restricted cone property.

Theorem XI.81 Let Γ be a closed bounded set of measure zero in $\mathbb{R}^3$. Write $\mathbb{R}\backslash\Gamma = \Lambda_1 \cup \Lambda_2$ where Λ_1 is the unbounded component and Λ_2 the union of the bounded components. Suppose that Λ_1 and Λ_2 have the restricted cone property. Then for any open ball containing Γ, $\tilde{R}_{\partial B \cup \Gamma;N}^2$ is trace class.

In this appendix we prove Theorems XI.79 and 80 and sketch a proof of Theorem XI.81 in the special case where Γ is the union of the boundaries of a finite number of starlike regions with smooth boundary. The general case of Theorem XI.81, which is proven by very different methods, can be found in the reference in the Notes.

In the proofs of Theorems XI.79 and 80, we need various properties of R_0, $R_{\Gamma;D}$, $R_{\Gamma;N}$ established in Chapter XIII or by the methods of that chapter. We summarize the results that we need:

Lemma 1 Let Γ be fixed and B be a fixed ball containing Γ. Then:

(a) As operator inequalities on $L^2(\mathbb{R}^3)$,

$$R_{\Gamma;D} \leq R_0 \leq R_{\Gamma;N} \leq R_{\partial B \cup \Gamma;N}$$

(b) Under the direct sum decomposition $L^2(\mathbb{R}^3) = L^2(B) \oplus L^2(\mathbb{R}^3\backslash B)$, $R_{\partial B \cup \Gamma;N} = \tilde{R}_{\partial B \cup \Gamma;N} \oplus R'$ for suitable R'.

(c) R_0, $R_{\Gamma;D}$, and $R_{\Gamma;N}$ are contractions from $L^\infty(\mathbb{R}^3)$ to itself.

Proof (a) In a suitable sense of $\leq$ for unbounded operators, $H_{\Gamma \cup \partial B;N} \leq H_{\Gamma;N} \leq H_0 \leq H_{\Gamma;D}$ (see Proposition 4 of Section XIII.15) from which (a) follows by general principles (Problem 117).

(b) This is just Proposition 3 of Section XIII.15.

(c) By the second Beurling–Deny criterion (Theorem XIII.51), $e^{-tH_{\Gamma;D}}$ is a contraction on L^∞ (see Example 3, revisited, in Appendix 1 to Section XIII.12) and thus since

$$R_{\Gamma;D} = \int_0^\infty e^{-t} e^{-tH_{\Gamma;D}}\, dt$$

so is $R_{\Gamma;D}$. A similar proof works for R_0 and $R_{\Gamma;N}$. ∎

Lemma 2 If $(1 + x^2)(R_0 - R_{\Gamma;D})(1 + x^2)$ is Hilbert–Schmidt, then $R_0^2 - R_{\Gamma;D}^2$ is trace class. Similarly, if $(1 + x^2)(R_0 - R_{\Gamma;N})(1 + x^2)$ is Hilbert–Schmidt, then $R_0^2 - R_{\Gamma;N}^2$ is trace class.

Proof Write

$$R_0^2 - R_{\Gamma;D}^2 = R_0(R_0 - R_{\Gamma;D}) + (R_0 - R_{\Gamma;D})R_0 - (R_0 - R_{\Gamma;D})^2$$

By Theorem XI.21 or by explicit calculation from the integral kernel $4\pi|x - y|^{-1}e^{-|x-y|}$ of R_0, $R_0(1 + x^2)^{-1}$ is Hilbert–Schmidt. Thus, to prove that $R_0^2 - R_{\Gamma;D}^2$ is trace class, it suffices that $(1 + x^2)(R_0 - R_{\Gamma;D})$ and $(R_0 - R_{\Gamma;D})$ be Hilbert–Schmidt and this follows from the hypotheses. The Neumann case is similar. ∎

Lemma 3 Let $K \geq 0$ and let C and D be bounded operators with $C + D = I$. Then K is Hilbert–Schmidt if and only if C^*KC and D^*KD are Hilbert–Schmidt. In particular, if χ is the characteristic function of a bounded set Ω and both

$$\chi(R_0 - R_{\Gamma;D})\chi \quad \text{and} \quad (1 + x^2)(1 - \chi)(R_0 - R_{\Gamma;D})(1 - \chi)(1 + x^2)$$

respectively,

$$\chi(R_{\Gamma;N} - R_0)\chi \quad \text{and} \quad (1 + x^2)(1 - \chi)(R_{\Gamma;N} - R_0)(1 - \chi)(1 + x^2)$$

are Hilbert-Schmidt, then $R_0^2 - R_{\Gamma;D}^2$ [respectively, $(R_0^2 - R_{\Gamma;N}^2)$] is trace class.

Proof For K to be in $\mathscr{I}_2$, it is necessary and sufficient that $K^{1/2}$ be in $\mathscr{I}_4$. But this happens if and only if both $K^{1/2}C$ and $K^{1/2}D$ are in $\mathscr{I}_4$. This proves the first part of the lemma.

The last part of the lemma follows from the first part, Lemma 2 and Lemma 1a, which implies that $R_{\Gamma;N} - R_0$ and $R_0 - R_{\Gamma;D}$ are nonnegative operators. ∎

$R_{\Gamma;D}$ defines a bilinear form on $\mathscr{S} \times \mathscr{S}$ by $\langle \varphi, \psi \rangle \mapsto (\bar{\varphi}, R_{\Gamma;D}\psi)$ and, so by the nuclear theorem (Theorem V.12) there is a distribution $G_{\Gamma;D}(x, y)$, called the **Dirichlet Green's function** so that

$$(\varphi, R_{\Gamma;D}\psi) = \int \bar{\varphi}(x)\psi(y)G_{\Gamma;D}(x, y)\,dx\,dy$$

for $\varphi, \psi \in \mathscr{S}$. The **Neumann Green's function** $G_{\Gamma;N}(x, y)$ and **free Green's function** $G_0(x, y)$ are defined similarly. Of course,

$$G_0(x, y) = (4\pi)^{-1}|x - y|^{-1}e^{-|x-y|}$$

Lemma 4 Let B be an open ball containing Γ. Then $G_{\Gamma;D} - G_0$ and $G_{\Gamma;N} - G_0$ are C^∞ on $(\mathbb{R}^3\backslash\bar{B}) \times (\mathbb{R}^3\backslash\bar{B})$ and obey the estimates

$$|(G_{\Gamma;N} - G_0)(x, y)| \leq Ce^{-\frac{1}{2}|x|-\frac{1}{2}|y|} \tag{206a}$$

$$|(G_{\Gamma;D} - G_0)(x, y)| \leq Ce^{-\frac{1}{2}|x|-\frac{1}{2}|y|} \tag{206b}$$

In particular, if χ is the characteristic function of B, then

$$(1 + x^2)(1 - \chi)(R_0 - R_{\Gamma;D})(1 - \chi)(1 + x^2)$$

and

$$(1 + x^2)(1 - \chi)(R_{\Gamma;N} - R_0)(1 - \chi)(1 + x^2)$$

are Hilbert-Schmidt operators.

Proof We consider the Neumann case; the Dirichlet case is similar. Let $h, g \in C_0^\infty(\mathbb{R}^3\backslash\Gamma)$. Then $(H_{\Gamma;N} + 1)h = (-\Delta + 1)h$ so that

$$\iint \overline{[(-\Delta + 1)h](x)}\,G_{\Gamma;N}(x, y)g(y)\,dx\,dy = \int \overline{h(x)}\,g(x)\,dx$$

Therefore, as a distribution on $C_0^\infty((\mathbb{R}^3\backslash\Gamma) \times (\mathbb{R}^3\backslash\Gamma))$,

$$(-\Delta_x + 1)G_{\Gamma;N}(x, y) = \delta(x - y)$$

so that

$$(-\Delta_x - \Delta_y + 2)(G_{\Gamma;N}(x, y) - G_0(x, y)) = 0$$

It follows by elliptic regularity (Theorem IX.25) that $Q(x, y) \equiv G_{\Gamma;N}(x, y) - G_0(x, y)$ is C^∞ on $(\mathbb{R}^3\backslash\Gamma) \times (\mathbb{R}^3\backslash\Gamma)$ and, in particular, on $(\mathbb{R}^3\backslash\bar{B}) \times (\mathbb{R}^3\backslash\bar{B})$. We first claim that for $x, y \in \mathbb{R}^3\backslash\bar{B}$,

$$Q(x, y) = \int_{z \in \partial B} \left[\frac{Q(z, y)}{\partial n_z} G_0(z, x) - Q(z, y)\,\frac{\partial G_0}{\partial n_z}(z, x)\right] d\Omega_z \tag{207}$$

where $d\Omega$ is the surface measure on ∂B and n_z is the normal to B pointing outward from B at z.

Let $\tilde{B}$ be a sphere of very large radius enclosing ∂B, x, and y. Then (207) with $\int_{z \in \partial B}$ replaced by $\int_{z \in \partial B} - \int_{z \in \partial\tilde{B}}$ follows from $(-\Delta_x + 1)Q(x, y) = 0$ and $(-\Delta_x + 1)G_0(x, y) = \delta(x - y)$ by a standard argument using Green's formula

$$\int_\Omega (h\,\Delta g - g\,\Delta h)\,dx = \int_{\partial\Omega} (h\,\partial g/\partial n - g\,\partial h/\partial n)\,d\sigma$$

Thus (207) follows if we can show that the $\partial\tilde{B}$ integral goes to zero as $\partial\tilde{B}$ goes to ∞. Actually, we need only prove a weaker statement, namely, suppose we can prove that the $\partial\tilde{B}$ integral goes to zero as $r_0 \to \infty$ after we integrate over y with some $h \in C_0^\infty$ and integrate the radius of $\partial\tilde{B}$ from r_0 to $r_0 + 1$. Then by integrating the Green's formula result over the radius of $\partial\tilde{B}$ and taking $r_0 \to \infty$, we obtain (207) with y smeared out. We can then take h to a δ-function and obtain (207).

In the integral over the radius of $\partial\tilde{B}$, we can integrate the $\partial Q/\partial n_z$ by parts and so obtain an error term involving only G_0, $\partial G_0/\partial n_z$, and Q (no $\partial Q/\partial n_z$). Since G_0 and $\partial G_0/\partial n$ have exponential falloff as $|x - z| \to \infty$, it is sufficient to prove that $\int Q(z, y)h(y)\,dy$ is bounded as $z \to \infty$. But this follows from Lemma 1c! As a result, (207) holds for ∂B the boundary of any ball containing Γ.

Choose balls B_1 and B_2 with $\Gamma \subset B_1$, $\bar{B}_1 \subset B_2$, $\bar{B}_2 \subset B$. Now, since Q is C^∞ on $(\mathbb{R}^n\backslash\Gamma) \times (\mathbb{R}^n\backslash\Gamma)$, it follows that Q, $\nabla_x Q$, $\nabla_y Q$, and $\nabla_x\nabla_y Q$ are uniformly bounded on $\bar{B}_2\backslash B_1$ and, so by (207) with B replaced by B_1, Q and $\nabla_y Q$ are uniformly bounded for $x \in \mathbb{R}^3\backslash B$ and $y \in B_2$. By the symmetry of Q, we have that Q and $\nabla_x Q$ are uniformly bounded for $x \in B_2$ and $y \in \mathbb{R}^3\backslash B$. Using (207) with B replaced by B_2, this uniform bound, the exponential falloff of G_0, and the symmetry of Q, we obtain (206). ∎

Proof of Theorem XI.79 Since $0 \leq R_0 - R_{\Gamma;D} \leq R_0$ by Lemma 1a, it suffices to prove that $\chi R_0 \chi$ is Hilbert-Schmidt to conclude that

$\chi(R_0 - R_{\Gamma;D})\chi \in \mathscr{I}_2$ and thereby complete the proof by Lemmas 3 and 4. But $\chi R_0 \chi \in \mathscr{I}_2$ by direct calculation from the formula for G_0 or by Theorem XI.21. ∎

Proof of Theorem XI.80 By Lemma 1a,

$$0 \leq R_{\Gamma;N} - R_0 \leq R_{\Gamma;N} \leq R_{\Gamma \cup \partial B;N}$$

and by Lemma 1b, $\chi R_{\partial B \cup \Gamma;N}\chi = \tilde{R}_{\partial B \cup \Gamma;N} \oplus 0$ which is Hilbert–Schmidt by hypothesis. The theorem now follows from Lemmas 3 and 4. ∎

We now sketch a proof of Theorem XI.81 in a special case, leaving the details to the reader:

Lemma 5 Let $\Omega \subset B \subset \mathbb{R}^3$ be open balls with center 0. Let $\Gamma = \partial\Omega$, $S = \partial B$. Then $\tilde{R}_{\Gamma \cup S;N}$, the operator on $L^2(B)$ with Neumann boundary conditions on Γ and S, is Hilbert–Schmidt.

Proof By Lemma 1b, $\tilde{R}_{\Gamma \cup S;N} = R_1 \oplus R_2$ under the decomposition $L^2(B) = L^2(\Omega) \oplus L^2(B\backslash\Omega)$. We consider the R_1 case; the R_2 case is similar. $\tilde{H}_{\Gamma;N}$ is a direct sum $\oplus_{\ell,m} \tilde{h}_{\ell,m}$ of operators under the decomposition $L^2(B) = \oplus \tilde{\mathscr{H}}_{\ell,m}$ where $\tilde{\mathscr{H}}_{\ell m} = \{\psi(r)Y_{\ell m}(\theta, \varphi)\}$. Under the isomorphism $\psi(r)Y_{\ell m} \leftrightarrow r\psi \equiv f$, $\tilde{\mathscr{H}}_{\ell m}$ goes over to $L^2(0, a)$ where $a = \text{rad}(\Omega)$, and $\tilde{h}_{\ell m}$ to

$$h_{\ell m} = -d^2/dr^2 + \ell(\ell + 1)r^{-2}$$

with boundary conditions

$$f(0) = 0, \qquad a^2(r^{-1}f)'(a) = af'(a) - f(a) = 0$$

One can therefore find explicitly the eigenfunctions of $h_{0,0}$ in terms of trigonometric functions and find that the nth eigenvalue obeys $E_{n,\ell=0} \geq C_1 n^2$. Since $h_{\ell m} \geq h_{0,0} + \ell(\ell + 1)a^{-2}$, $E_{n,\ell} \geq C(n^2 + \ell^2)$, so

$$\sum_{n=0}^{\infty} (E_{n,\ell} + 1)^{-2} \leq d_1 \int_0^{\infty} (x^2 + \ell^2 + 1)^{-2}\, dx = d(\ell^2 + 1)^{-3/2}$$

Thus

$$\text{Tr}(R_1^2) = \sum_{\ell=0}^{\infty} (2\ell + 1) \sum_{n=0}^{\infty} (E_{n,\ell} + 1)^{-2} < \infty \quad ∎$$

Lemma 6 Let Γ_1 and Γ_2 be two closed sets of measure zero respectively inside bounded open sets Ω_1, Ω_2 in $\mathbb{R}^3$. Let $S_i = \partial\Omega_i$. Suppose that there

exists a C^∞ diffeomorphism F of a neighborhood of $\bar{\Omega}_1$ to a neighborhood of $\bar{\Omega}_2$ so that $F[\Omega_1] = \Omega_2$ and $F[\Gamma_1] = \Gamma_2$. Then $\tilde{R}_{\Gamma_1 \cup S_1;N}$ is Hilbert–Schmidt if and only if $\tilde{R}_{\Gamma_2 \cup S_2;N}$ is Hilbert–Schmidt.

Proof Consider the unitary map $U: L^2(\Omega_2, d^3x) \to L^2(\Omega_1, d^3x)$ given by

$$(Uf)(x) = (G^{1/2}f)(Fx)$$

where $G = \det\{J_{ij}\}$ and $J_{ij} = \{\partial F_i(x)/\partial x_j\}$. Then

$$U\tilde{H}_{\Gamma_2 \cup S_2;N}U^{-1} = H'$$

where H' has the same form domain as $\tilde{H}_{\Gamma_1 \cup S_1;N}$ and

$$\begin{aligned}(f, H'f) &= \int_{\Omega_1} \sum_i \left| \sum_j (J^{-1})_{ij} \frac{\partial(G^{1/2}f)}{\partial x_j} \right|^2 d^3x \\ &\leq C_1 \int_{\Omega_1} \sum_i \left| \frac{\partial f}{\partial x_i} \right|^2 + |f|^2\, d^3x \\ &= C_1(f, (H_{\Gamma_1 \cup S_1;N} + 1)f)\end{aligned}$$

It follows that (Problem 117)

$$\tilde{R}_{\Gamma_1 \cup S_1;N} \leq C_2(H' + 1)^{-1}$$

so that $\tilde{R}_{\Gamma_1 \cup S_1;N}$ is Hilbert–Schmidt if $(H' + 1)^{-1}$ is Hilbert–Schmidt. Since H' is unitarily equivalent to $\tilde{H}_{\Gamma_2 \cup S_2;N}$, we see that $\tilde{R}_{\Gamma_1 \cup S_1;N} \in \mathscr{I}_2$ if $\tilde{R}_{\Gamma_2 \cup S_2;N} \in \mathscr{I}_2$. By symmetry, we can go in the other direction. ∎

Definition An open set Ω in $\mathbb{R}^3$ is called **starlike about** x_0 in Ω if for any unit vector n, $\Omega \cap \{x_0 + tn \,|\, t \in [0, \infty)\} = \{x_0 + tn \,|\, t \in [0, a_n)\}$ for some $a_n > 0$. If a_n is a C^∞ function of n, we say that Ω has a **smooth boundary**.

Lemma 7 Let Γ_1 be the boundary of an open set D_1 that is starlike with smooth boundary with respect to x_0. Let

$$\Omega_1 = \{y \,|\, x_0 + (1 + \varepsilon)^{-1}(y - x_0) \in D_1\}$$

for some fixed $\varepsilon > 0$. Then, there is a C^∞ diffeomorphism F of a neighborhood of $\bar{\Omega}_1 \supset D_1$ onto a neighborhood of a ball $\bar{\Omega}_2$ such that $F[\Omega_1] = \Omega_2$ and such that $\Gamma_2 \equiv F[\Gamma_1]$ is the boundary of a sphere in Ω_2 with the same center as Ω_2. In particular, $\tilde{R}_{\Gamma_1 \cup S_1;N}$ is Hilbert–Schmidt.

Proof Just define $F(x) = (x - x_0)a_{n(x)}^{-1}$ where $n(x) = (x - x_0)\,|x - x_0|^{-1}$. ∎

Finally, we can prove a special case of Theorem XI.81.

Theorem XI.81′ Let Γ be the union of a finite number of disjoint sets $\{\Gamma_j\}_{j=1}^k$ each of which is the smooth boundary of a bounded open starlike set Ω_j. Let B be any open ball containing Γ and let $S = \partial B$. Then $\tilde{R}_{\Gamma \cup S;N}$ is Hilbert–Schmidt.

Proof Let x_j be the point about which Ω_j is starlike. Let S_j be Γ_j scaled outward slightly from x_j. This can be done so that the S_j are disjoint and contained inside B. Let S' be the surface of a sphere concentric to S, inside S, and containing all the S_i (see Figure XI.13). Let $\chi_1, \ldots, \chi_k$ be the characteristic functions of the regions surrounded by the $S_j, j = 1, \ldots, k$. Let χ_{k+1} be

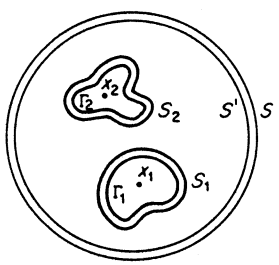


FIGURE XI.13 The sets S_i and S.

the characteristic function of the shell between S and S' and let χ_0 be the characteristic function of the rest of B so that $\sum_{j=0}^{k+1} \chi_j \equiv 1$ on B. Then, by an extension of Lemma 3, it suffices to prove that $\chi_j R_{\Gamma \cup S;N} \chi_j$ is Hilbert–Schmidt for each $j = 0, 1, \ldots, k+1$. The case $j = 0$ is trivial since $G_{\Gamma \cup S;N}(x, y) - G_0(x, y)$ is C^∞ on $\overline{\text{supp } \chi_0} \times \overline{\text{supp } \chi_0}$ by Lemma 4 and $\chi_0(x)G_0(x, y)\chi_0(y)$ is the kernel of a Hilbert–Schmidt operator. For $j = 1, \ldots, k$,

$$\chi_j \tilde{R}_{\Gamma \cup S;N} \chi_j \leq \chi_j \tilde{R}_{\Gamma \cup S_j \cup S;N} \chi_j = \tilde{R}_{\Gamma_j \cup S_j;N} \oplus 0$$

by Lemmas 1a and 1b. By Lemma 7, $\tilde{R}_{\Gamma_j \cup S_j;N}$ is Hilbert–Schmidt so $\chi_j \tilde{R}_{\Gamma \cup S;N} \chi_j$ is Hilbert–Schmidt too. The case $j = k + 1$ is similar. ∎

XI.11 Optical and acoustical scattering II: The Lax–Phillips method

In this section we study a different approach to scattering theory developed by Lax and Phillips—different in that the main objects of study are certain families of subspaces of the Hilbert space of the interacting dynamics. As we shall see, this approach applies most naturally to classical

wave equations that obey Huygens' principle rather than to quantum mechanics where the wave equations are dispersive and have infinite propagation speed. Nevertheless, by using the principle of invariance of the wave operators, it can also be applied in some quantum-mechanical situations (see Example 5).

The most beautiful and important aspect of the Lax–Phillips approach is that certain analyticity properties of the scattering operator arise naturally. When the interacting group satisfies the basic hypotheses of the theory, then there is a unitary map from $\mathscr{H}$ to $L^2(\mathbb{R}; N)$ where N is an auxiliary Hilbert space. In this representation of $\mathscr{H}$, the scattering operator acts by multiplication by an $\mathscr{L}(N)$-valued function $s(\sigma)$ which is unitary a.e. and which is the boundary value of an analytic $\mathscr{L}(N)$-valued function $s(z)$ in the upper half-plane. Typically, $s(z)$ can be meromorphically continued to the lower half-plane, and its poles are closely tied to the geometry and to the physical interpretation of the theory. We have already had examples of such continuations in Sections 7 and 8 and the appendix to Section 6.

A complete exposition of the Lax–Phillips theory is beyond the scope of this section. What we wish to do is to prove several of the basic theorems so that the underlying structure and the origin of the above-mentioned analyticity are clear. We then sketch several examples to show how the hypotheses are proven in practice. Detailed expositions and many applications can be found in the references discussed in the Notes.

The basic idea which is isolated and developed in the Lax–Phillips theory is that of incoming and outgoing subspaces.

Definition Let $U(t)$ be a strongly continuous unitary group on a Hilbert space $\mathscr{H}$. A closed subspace $D_+ \subset \mathscr{H}$ is said to be **outgoing** if:

(i) $U(t)[D_+] \subset D_+$ for $t \geq 0$.
(ii) $\bigcap_t U(t)[D_+] = \{0\}$.
(iii) $\overline{\bigcup_t U(t)[D_+]} = \mathscr{H}$.

Similarly, if D_- satisfies (ii), (iii) and

(i′) $U(t)[D_-] \subset D_-$ for $t \leq 0$,

then D_- is said to be **incoming**.

This terminology arose naturally in applications. For instance, in the Hilbert space for the free wave equation on $\mathbb{R}^3$ (see Example 1), D_+ is just the set of initial data so that the solution $u(x, t)$ vanishes if $|x| \leq t$; that is, physically, the waves are going out in the future. Similarly, D_- is the set of

initial data so that $u(x, t)$ vanishes if $|x| \leq -t$. Such a solution is coming in in the past.

An example of an outgoing subspace can be constructed as follows. Let N be a Hilbert space, let $\mathscr{H} = L^2(\mathbb{R}; N)$, and define $U(t)$ to be translation to the right by t units, that is, $(U(t)f)(s) = f(s - t)$. Then

$$D_+ = L^2(0, \infty; N) \equiv \{f \in L^2(\mathbb{R}; N) \mid f(s) = 0 \text{ for } s < 0\}$$

is outgoing. The main structure theorem of this section says that in fact all outgoing subspaces are essentially of this form.

Theorem XI.82 Let $U(t)$ be a strongly continuous unitary group on a Hilbert space $\mathscr{H}$ and let D_+ be an outgoing subspace for $U(t)$. Then there is an auxiliary Hilbert space N and a unitary map $\mathscr{R}_+$ of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ so that $\mathscr{R}_+[D_+] = L^2(0, \infty; N)$ and $U_+(t) \equiv \mathscr{R}_+ U(t)\mathscr{R}_+^{-1}$ is translation to the right by t units. Similarly, if D_- is an incoming subspace, there is a unitary map $\mathscr{R}_-$ onto $L^2(\mathbb{R}; N')$ so that $\mathscr{R}_-[D_-] = L^2(-\infty, 0; N')$ and $U_-(t) \equiv \mathscr{R}_- U(t)\mathscr{R}_-^{-1}$ is translation to the right by t units. If $U(t)$ has both incoming and outgoing subspaces, N and N' can be chosen to be the same, although $\mathscr{R}_+$ may not equal $\mathscr{R}_-$. These representations are unique up to isomorphisms of N.

$U_+(t)$, $L^2(0, \infty; N)$, and $L^2(\mathbb{R}; N)$ are said to be an **outgoing translation representation** of $U(t)$, D_+, and $\mathscr{H}$. Similarly, $U_-(t)$, $L^2(-\infty, 0; N)$, and $L^2(\mathbb{R}; N)$ are said to be an **incoming translation representation** of $U(t)$, D_-, and $\mathscr{H}$.

Before proving the theorem, we make several remarks. First, if $U(t)$ has incoming and outgoing subspaces, we can construct a scattering operator as follows. For $\varphi \in \mathscr{H}$, let $\varphi_- = \mathscr{R}_- \varphi$ and $\varphi_+ = \mathscr{R}_+ \varphi$, and define $\tilde{S}$ to be the map $\tilde{S}$: $\varphi_- \mapsto \varphi_+$, that is,

$$\tilde{S} = \mathscr{R}_+ \mathscr{R}_-^{-1}$$

$\tilde{S}$ is a unitary map from $L^2(\mathbb{R}; N)$ to itself. S is defined by pulling this operator back to $\mathscr{H}$:

$$S \equiv \mathscr{R}_-^{-1}(\mathscr{R}_+ \mathscr{R}_-^{-1})\mathscr{R}_- = \mathscr{R}_-^{-1}\mathscr{R}_+$$

Finally, letting $\mathscr{F}$ denote the Fourier transform, a unitary map from $L^2(\mathbb{R}; N)$ to itself, we define

$$\hat{S} \equiv \mathscr{F}\tilde{S}\mathscr{F}^{-1}$$

S, $\hat{S}$, and $\tilde{S}$ are clearly unitarily equivalent, so we shall call them all **the scattering operator**, distinguishing between the representations by the $\hat{}$ and $\tilde{}$.

Since $\mathscr{R}_\pm U(t) = U_\pm(t)\mathscr{R}_\pm$ and $U_+(t) = U_-(t)$, S commutes with $U(t)$. Since $\tilde{S}$ commutes with translation, it should intuitively be given by convolution by an $\mathscr{L}(N)$-valued function τ on $\mathbb{R}$, so $\hat{S}$ should be given by multiplication by an operator-valued function $s = (2\pi)^{1/2}\hat{\tau}$. If we have the additional hypothesis that $D_- \subset D_+^\perp$, then $\tilde{S}$ takes $L^2(-\infty, 0; N)$ into itself, which requires that τ have support on $(-\infty, 0]$. The Paley–Wiener theorem thus suggests that s should have an analytic extension to the upper half-plane. This is the source of the analyticity described in the introductory remarks above (details are given in Theorem XI.89 and its corollary).

Notice that the definition of the scattering operator did not mention any "free dynamics." In practice, the incoming and outgoing subspaces are constructed by using the free dynamics; and $\mathscr{R}_+$ and $\mathscr{R}_-$ turn out to be (unitarily equivalent to) the usual wave operators. This is further discussed below. However, the construction above raises the possibility of defining S when there is no "natural" candidate for the free dynamics or in situations where the convergence of interacting solutions to free solutions as $t \to \pm\infty$ is too slow to allow the usual construction of the wave operators. However, we emphasize that the construction does depend on more than the interacting dynamics $U(t)$. For example, once one has an outgoing translation representation of $\mathscr{H}$ as $L^2(-\infty, \infty; N)$, one can take $\tilde{D}_- = \mathscr{R}_+^{-1}[L^2(-\infty, 0; N)]$. For the pair D_+, $\tilde{D}_-$, the S-matrix is I. Typically, the additional structure that determines the choice of D_+ and D_- is some underlying geometry.

One inherent restriction of the theory as it stands is apparent from Theorem XI.82 itself. The existence of an incoming or outgoing translation representation for $U(t)$ implies that its generator H has purely absolutely continuous spectrum on the whole real axis and that the spectrum has uniform multiplicity. This, however, does not make applications to quantum mechanics impossible (see Example 5).

As motivation for our proof of Theorem XI.82, we first prove the discrete analogue.

Theorem XI.83 Let V be a unitary operator on a separable Hilbert space $\mathscr{H}$. Let D_+ be a closed subspace of $\mathscr{H}$ so that:

(i) $V[D_+] \subset D_+$.
(ii) $\bigcap_{k \in \mathbb{Z}} V^k[D_+] = \{0\}$.
(iii) $\overline{\bigcup_{k \in \mathbb{Z}} V^k[D_+]} = \mathscr{H}$.

Then there is a Hilbert space N and a unitary map $\imath_+$ of $\mathscr{H}$ onto $\ell_2(-\infty, \infty; N)$ such that

$$\imath_+[D_+] = \{f \mid f(n) = 0, n < 0\} \equiv \ell_2[0, \infty; N)$$

and $\tilde{V} = \iota_+ V \iota_+^{-1}$ is the right shift. This representation is unique up to isomorphism of N.

Proof We prove the existence of ι_+ and leave uniqueness to the reader (Problem 121). Let $N = D_+ \cap (V[D_+])^\perp$ which is a closed subspace of $\mathscr{H}$. Since V is unitary,

$$VN = VD_+ \cap V^2 D_+^\perp \subset VD_+ \subset N^\perp$$

so we can form the direct sum $N \oplus VN$. Since $N \oplus VD_+ = D_+$, we have $VN \oplus V^2 D_+ = VD_+$ so that

$$N \oplus VN \oplus V^2 D_+ = D_+$$

or equivalently,

$$N \oplus VN = D_+ \cap V^2 D_+^\perp$$

In the same way one sees inductively that

$$V^j N \subset V^j D_+ \subset (N \oplus \cdots \oplus V^{j-1} N)^\perp$$

$$N \oplus \cdots \oplus V^j N = D_+ \cap V^{j+1} D_+^\perp \tag{208}$$

By (i), $D_+ \supseteq VD_+ \supseteq \cdots \supseteq V^j D_+$ so by (ii) and (208):

$$\bigoplus_{k \geq 0} V^k N = D_+ \tag{209}$$

Applying V^{-1} to $N \oplus VD_+ = D_+$, we see that

$$V^{-1} N \oplus D_+ = V^{-1} D_+$$

so that inductively one sees that

$$\bigoplus_{k \geq \ell} V^k N = V^\ell D_+$$

for ℓ any integer, positive or negative. Taking $\ell \to -\infty$ and using (iii), we see that

$$\bigoplus_{k \in \mathbb{Z}} V^k N = \mathscr{H}$$

Thus any $\varphi \in \mathscr{H}$ can be uniquely written

$$\varphi = \sum_k V^k \varphi_k, \qquad \varphi_k \in N$$

with $\|\varphi\|^2 = \sum_k \|\varphi_k\|^2$. As a result, the map

$$\varphi \xrightarrow{\iota_+} \{\varphi_k\}_{k=-\infty}^{\infty}$$

is a unitary map of $\mathscr{H}$ onto $\ell_2(-\infty, \infty; N)$. By (209), $\iota_+ D_+ = \ell_2[0, \infty; N)$, and it is easy to check that $\tilde{V}$ is the right shift. ∎

There are at least three fairly distinct proofs of Theorem XI.82. One reverses the analysis of Theorem XI.84 below and uses von Neumann's uniqueness theorem to prove Theorem XI.82. The second uses techniques of Fourier analysis, Theorem XI.83, and the Cayley transform. The proof we give depends on spectral multiplicity theory (see Section VII.2) and has its roots in general group theoretic methods, especially Mackey's imprimitivity theorem. We recall that two measures are called **equivalent** if and only if they are mutually absolutely continuous. The key technical result we need in our proof of Theorem XI.82 is closely connected to the fact that Lebesgue measure is the unique translation invariant measure on $\mathbb{R}$ (Problem 122).

Lemma Suppose that $d\mu$ is a nontrivial Borel measure on $\mathbb{R}$ with the property that $d\mu(\cdot + a)$ is equivalent to $d\mu$ for all $a \in \mathbb{R}$. Then $d\mu$ is equivalent to Lebesgue measure.

Proof By hypothesis

$$d\mu(x + y) = g_y(x)\, d\mu(x) \tag{210}$$

It is immediate that $g_y(x)$ is measurable in x for each fixed y and $\int h(x) g_y(x)\, d\mu(x) = \int h(x - y)\, d\mu(x)$ is measurable in y for each measurable h, and thus $g_y(x)$ is jointly measurable.

Fix $h \geq 0$ with $\int h(y)\, dy = 1$ and let f be a simple function. Then, freely using Fubini's theorem:

$$\alpha \equiv \int f(x)\, d\mu(x) = \iint f(x) h(y)\, d\mu(x)\, dy$$

$$= \iint f(x + y) g_y(x) h(y)\, d\mu(x)\, dy \tag{211}$$

by (210). Make the change of variables $z = x + y$ for fixed x, so that

$$\int f(x + y) g_y(x) h(y)\, dy = \int f(z) g_{z-x}(x) h(z - x)\, dz$$

by the translation invariance of Lebesgue measure. Thus

$$\alpha = \int f(z) G(z)\, dz$$

where

$$G(z) = \int g_{z-x}(x)h(x - z)\, d\mu(x)$$

Since f is arbitrary,

$$d\mu(x) = G(x)\, dx$$

Now, fix $h \geq 0$ with $\int h(y)\, d\mu(y) = 1$ and compute, as above, that

$$\int f(x)\, dx = \iint f(x)h(y)\, d\mu(y)\, dx$$

$$= \iint f(x + y)h(y)\, dx\, d\mu(y)$$

$$= \iint f(z)h(z - x)g_{-x}(z)\, d\mu(z)\, dx$$

$$= \int f(z)H(z)\, d\mu(z)$$

with $H(z) = \int h(z - x)g_{-x}(z)\, dx$. Thus

$$dx = H(x)\, d\mu(x) \quad \blacksquare$$

Proof of Theorem XI.82 Motivated by the proof of Theorem XI.83, we define

$$D_+(t) \equiv U(t)[D_+], \qquad t \in \mathbb{R}$$

$$D_+(\infty) \equiv \{0\}, \qquad D_+(-\infty) \equiv \mathscr{H}$$

and for $a < b$ we define

$$N(a, b] = D_+(a) \cap D_+(b)^\perp$$

Let $P_{(a,b]}$ be the orthogonal projection onto $N(a, b]$. Then from properties (i)–(iii) of D_+ and the fact that $U(t)$ is continuous, it is easy to check that $\{P_{(a,b]}\}$ generates a projection-valued measure $\{P_\Omega\}$ that satisfies $U(t)P_\Omega U(-t) = P_{\Omega+t}$. Introducing the operator

$$X = \int_{\mathbb{R}} \lambda\, dP_\lambda$$

this implies that $U(t)XU(t)^{-1} = X + t$. It follows from the uniqueness of the spectral multiplicity measure classes (Theorem VII.6) that the spectral measure classes of X are invariant under translation. Thus, by the lemma, each

class must be the one containing Lebesgue measure. Since the measure classes are disjoint, there is only one measure class, that is, X is a self-adjoint operator of uniform multiplicity m for some m with corresponding measure dx. It follows that there is a Hilbert space N of dimension m and a unitary map $\mathscr{Q}_+ : \mathscr{H} \to L^2(\mathbb{R}, dx; N)$ so that $\mathscr{Q}_+ P_\Omega \mathscr{Q}_+^{-1}$ is multiplication by χ_Ω, the characteristic function of Ω.

Let $W(t) = \mathscr{Q}_+ U(t)\mathscr{Q}_+^{-1}$ and let $T_0(t)$ be translation to the right by t units on $L^2(\mathbb{R}, dx; N)$. Then, for each t, $W(t)T_0(t)^{-1}$ commutes with each P_Ω; so by Theorem XIII.84, there is an $\mathscr{L}(N)$-valued measurable function $K_t(s)$ such that

$$(W(t)T_0(-t)f)(s) = K_t(s)f(s)$$

$K_t(s)$ is defined only almost everywhere in s, but for definiteness we make a choice for all s. Then

$$(W(t)f)(s) = K_t(s)f(t + s)$$

The group property $W(t)W(u) = W(t + u)$ implies that

$$K_t(s)K_u(t + s) = K_{t+u}(s) \tag{212}$$

(212) holds in the following sense: For each t and u, it holds for almost all s. Thus it holds for almost all triples $\langle s, t, u\rangle$, so we can choose a fixed value of s so that (212) holds for almost all $\langle t, u\rangle$. For that fixed value of s, define

$$(Bf)(t) = K_{t-s}(s)f(t)$$

Then

$$(BW(a)B^{-1}f)(t) = K_{t-s}(s)K_a(t)[K_{t+a-s}(s)]^{-1}f(t + a)$$

$$= f(t + a)$$

for almost all t and a where we have used (212) with the change of variables $t' = t + s$, $u' = a$. It follows that $BW(a)B^{-1} = T_0(a)$ for almost all a, and so by continuity for all a. Letting $\mathscr{R}_+ = B\mathscr{Q}_+$, the theorem results. ∎

Theorem XI.82 can be used to provide a proof of von Neumann's theorem (Theorem VIII.14) on the uniqueness of representations of the canonical commutation relations.

Theorem XI.84 (von Neumann's theorem) Let $U(t)$ and $V(s)$ be two strongly continuous one-parameter groups on a Hilbert space $\mathscr{H}$ that satisfy

$$U(t)V(s) = e^{its}V(s)U(t) \qquad \text{all } t \text{ and } s$$

Then there is a Hilbert space N and a unitary map $\mathscr{R}$ from $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ so that $\mathscr{R}U(t)\mathscr{R}^{-1}$ is translation to the right by t units and $\mathscr{R}V(s)\mathscr{R}$ is multiplication by $e^{-i\lambda s}$.

Proof Let P and Q be the self-adjoint operators with $U(t) = e^{-itP}$ and $V(s) = e^{-isQ}$. Let $\mathscr{D}$ denote the set of vectors in $\mathscr{H}$ of the form

$$\varphi_f = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(t, s)U(t)V(s)\varphi \, dt \, ds$$

where $\varphi \in \mathscr{H}$ and $f \in C_0^\infty(\mathbb{R}^2)$. Exactly as in the proof of Theorem VIII.8, one easily shows that $\mathscr{D}$ is dense in $\mathscr{H}$, $\mathscr{D} \subset D(Q)$, $\mathscr{D} \subset D(P)$, and that $\mathscr{D}$ is invariant under $U(s)$ and $V(t)$. By Theorem VIII.10, P and Q are essentially self-adjoint on $\mathscr{D}$. Let $\psi \in \mathscr{D}$, then since $U(t)\psi$ is in $\mathscr{D}$ also, we may differentiate both sides of the equality

$$U(t)V(s)\psi = e^{its}V(s)U(t)\psi$$

with respect to s. Setting $s = 0$, we obtain

$$U(t)QU(-t)\psi = (Q - tI)\psi \tag{213}$$

Since this relation is true on $\mathscr{D}$, which is a core for Q and $Q - tI$, we conclude that Q and $Q - tI$ are unitarily equivalent and (213) holds for all $\psi \in D(Q)$. Now, let $\{E_\Omega\}$ be the spectral family for Q. Then $\{U(t)E_\Omega U(-t)\}$ is the spectral family for $U(t)QU(-t)$. Since $E_\Omega = \chi_\Omega(Q)$, (213) implies that

$$U(t)E_{(-\infty, \lambda)}U(-t) = E_{(-\infty, \lambda+t)} \tag{214}$$

for all λ and t in $\mathbb{R}$.

Set $D_- = \text{Ran } E_{(-\infty, 0]}$. We shall show that D_- is an incoming subspace for $U(t)$ on $\mathscr{H}$. First, (214) implies that $U(t)D_- = \text{Ran } E_{(-\infty, \lambda+t]}$ for all t. Thus:

(i) $U(t)D_- \subset D_-$, $t \leq 0$;
(ii) $\bigcap_t U(t)D_- = \{0\}$;
(iii) $\overline{\bigcup_t U(t)D_-} = \mathscr{H}$;

by the usual properties of the spectral projections. So, by Theorem XI.82, there is an auxiliary Hilbert space N and a unitary map $\mathscr{R}_-$ of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ so that $\mathscr{R}_- D_- = L^2(-\infty, 0; N)$ and $\mathscr{R}_- U(t)\mathscr{R}_-^{-1}$ is translation to the right by t units. Finally, since $\mathscr{R}_- E_{(-\infty, 0)}\mathscr{R}_-^{-1} = \chi_{(-\infty, 0)}$, (214) implies that $\mathscr{R}_- E_{(-\infty, \lambda)}\mathscr{R}_-^{-1} = \chi_{(-\infty, \lambda)}$ for all λ. Thus $\mathscr{R}_- Q\mathscr{R}_-^{-1}$ is multiplication by λ and $\mathscr{R}_- e^{-iQs}\mathscr{R}_-^{-1}$ equals multiplication by $e^{-i\lambda s}$. ∎

Theorem XI.82 can be reformulated using the Fourier transform. Defined by the usual formula, the Fourier transform $\mathscr{F}$ is a unitary map of $L^2(\mathbb{R}; N)$ onto itself. It takes $L^2(0, \infty; N)$ onto the Hardy–Lebesgue class $\mathscr{H}_-^2(\mathbb{R}; N)$ and $L^2(-\infty, 0; N)$ onto $\mathscr{H}_+^2$ (see the Notes to Section IX.3).

Theorem XI.85 Let D_+ be an outgoing subspace for the unitary group $U(t)$ on a Hilbert space $\mathscr{H}$. Then there is an auxiliary Hilbert space N and a unitary map $\mathscr{F} \circ \mathscr{R}_+$ of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ such that $\mathscr{F} \circ \mathscr{R}_+[D_+] = \mathscr{H}_-^2(\mathbb{R}; N)$ and $(\mathscr{F} \circ \mathscr{R}_+)U(t)(\mathscr{F} \circ \mathscr{R}_+)^{-1}$ is multiplication by $e^{-i\sigma t}$.

The above representation is called an **outgoing spectral representation** for $U(t)$, D_+, and $\mathscr{H}$. For an incoming subspace a similar theorem holds except that $\mathscr{F} \circ \mathscr{R}_+$ is replaced by $\mathscr{F} \circ \mathscr{R}_-$ and $\mathscr{H}_-^2(\mathbb{R}; N)$ is replaced by $\mathscr{H}_+^2(\mathbb{R}; N)$.

The discussion after the statement of Theorem XI.82 shows that if we have incoming and outgoing subspaces, then we can construct a scattering theory. But, Theorem XI.82 says nothing about how one actually constructs incoming and outgoing subspaces for $U(t)$. Since $U(t)$ is the dynamics of an interacting system, this is not a trivial question. In applications, the construction depends heavily on the fact that $U(t)$ is closely related to a free dynamics $U_0(t)$ and that $U_0(t)$ has many special properties. For example, let $W_0(t)$ and $W(t)$ be the unitary groups for acoustical waves in free space and in inhomogeneous media constructed in the preceding section. Suppose that the region of inhomogeneity is contained inside some finite ball $\mathscr{B}_{r_0}$. The Hilbert spaces on which $W_0(t)$ and $W(t)$ act are equivalent, and the norms are equal for pairs of functions whose support lies outside $\mathscr{B}_{r_0}$. Furthermore, any data of compact support will eventually be propagated outside of $\mathscr{B}_{r_0}$ by $W_0(t)$; and as long as the data stay away from $\mathscr{B}_{r_0}$, $W_0(t)$ and $W(t)$ agree. These and other special properties of $W_0(t)$ and $W(t)$ are exploited in Examples 1 and 2 below. For the moment, we return to the general setting and formulate precisely what we mean by a "close relationship" between $U(t)$ and $U_0(t)$.

Suppose that $U(t)$ and $U_0(t)$ are strongly continuous unitary groups on Hilbert spaces $\mathscr{H}$ and $\mathscr{H}_0$ and let J be an identification operator from $\mathscr{H}_0$ to $\mathscr{H}$. Suppose that:

(0) There exist subspaces $D_\pm^{r_0} \subset \mathscr{H}_0 \cap \mathscr{H}$ so that the $\mathscr{H}_0$-norm and the $\mathscr{H}$-norm are the same on $D_\pm^{r_0}$ and J is the identity on $D_\pm^{r_0}$.
(1) $D_+^{r_0}$ and $D_-^{r_0}$ are incoming and outgoing for $U(t)$ *and* for $U_0(t)$.
(2) $U(t)$ and $U_0(t)$ act the same on $D_+^{r_0}$ for $t \geq 0$. $U(t)$ and $U_0(t)$ act the same on $D_-^{r_0}$ for $t \leq 0$.

(3) There is a Hilbert space N and a unitary map $\varphi \xrightarrow{\mathscr{R}_0} \tilde{\varphi}$ of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ so that $D^{r_0}_+$ and $D^{r_0}_-$ go over to $L^2(r_0, \infty; N)$ and $L^2(-\infty, -r_0; N)$, respectively, where r_0 is some positive number, and $U_0(t)$ goes over to translation by t. That is, up to a shift of r_0 units, this representation is both incoming *and* outgoing for $U_0(t)$.

Let $T_0(t)$ denote translation to the right on $L^2(\mathbb{R}; N)$. To construct an outgoing translation representation for $U(t)$, for each φ in $D^{r_0}_+$, we map $U(t)\varphi$ to $T_0(t)\tilde{\varphi}$. By (2), this map is well defined, it is norm preserving, and by (iii) it is densely defined. Further, it has dense range since $\mathscr{R}_0$ takes $D^{r_0}_+$ onto $L^2(r_0, \infty; N)$. The map thus extends to a unitary map of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ under which $U(t)$ goes over to T_0 and $D^{r_0}_+$ goes to $L^2(r_0, \infty; N)$. Left shift by $T_0(-r_0)$ makes this an outgoing translation representation for $U(t)$. A similar construction creates an incoming translation representation. We denote the maps onto the incoming and outgoing translation representations by $\mathscr{R}_+$ and $\mathscr{R}_-$ as before. Notice that, by (3), $D^{r_0}_+$ and $D^{r_0}_-$ are orthogonal. This will have important consequences later.

In this situation, where we have a free group $U_0(t)$, it is natural to ask how the Lax–Phillips scattering operator is related to the usual wave operators and scattering operator. Let D be the dense set of vectors φ in $\mathscr{H}_0$ so that $\mathscr{R}_0\varphi$ has compact support. If $\varphi \in D$, then for some s, $U_0(s)\varphi \in D^{r_0}_+$ so by (2), $U(-t)JU_0(t)\varphi$ is independent of t for $t \geq s$. Thus,

$$\Omega^-\varphi = \lim_{t\to\infty} U(-t)JU_0(t)\varphi$$

exists. Since D is dense, the limit exists on all of $\mathscr{H}_0$; a similar argument proves the existence of Ω^+.

Now, notice that if $\psi \in D^{r_0}_+$ then $\Omega^-\psi = \psi$; so if $\varphi \in D$ and $U_0(s_1)\varphi \in D^{r_0}_+$, then

$$\Omega^- U_0(s_1)\varphi = U_0(s_1)\varphi$$

Therefore,

$$\begin{aligned}\mathscr{R}_+\Omega^-\varphi = T_0(-s_1)\mathscr{R}_+\Omega^- U_0(s_1)\varphi &= T_0(-s_1)\mathscr{R}_+ U_0(s_1)\varphi \\ &= T_0(-r_0 - s_1)\mathscr{R}_0 U_0(s_1)\varphi \\ &= T_0(-r_0)\mathscr{R}_0\varphi\end{aligned}$$

since $\mathscr{R}_+ = T_0(-r_0)\mathscr{R}_0$ on $D^{r_0}_+$. Since such φ are dense, we have

$$\mathscr{R}_+\Omega^- = T_0(-r_0)\mathscr{R}_0$$

and similarly

$$\mathscr{R}_-\Omega^+ = T_0(r_0)\mathscr{R}_0$$

Since $\mathscr{R}_0$, $\mathscr{R}_\pm$, and $T_0(t)$ are unitary, this shows that Ran $\Omega^+ = \mathscr{H} =$ Ran Ω^-, so the wave operators are complete. Finally,

$$\begin{aligned}(\Omega^-)^{-1}\Omega^+ &= \mathscr{R}_0^{-1}T_0(r_0)\mathscr{R}_+\mathscr{R}_-^{-1}T_0(r_0)\mathscr{R}_0 \\ &= \mathscr{R}_0^{-1}T_0(r_0)\tilde{S}T_0(r_0)\mathscr{R}_0 \\ &= \mathscr{R}_0^{-1}(T_0(2r_0)\tilde{S})\mathscr{R}_0\end{aligned}$$

So, except for the inessential factor $T_0(2r_0)$, $(\Omega^-)^{-1}\Omega^+$ is just the Lax–Phillips scattering operator pulled back to $\mathscr{H}_0$. We summarize:

Theorem XI.86 Let $U_0(t)$, $U(t)$, and J satisfy the hypotheses (0)–(3) and let $\mathscr{R}_0$, T_0, and r_0 be defined as above. Then the wave operators $\Omega^\pm$ exist, are complete, and

$$(\Omega^-)^{-1}\Omega^+ = \mathscr{R}_0^{-1}(T_0(2r_0)\tilde{S})\mathscr{R}_0 \tag{215}$$

Example 1 (the free wave equation in three dimensions) We have already formulated the free wave equation as a Hilbert space problem in Sections X.13 and XI.10. We shall use the notation introduced in Section XI.10, setting $c_0 = 1$ by a suitable choice of units. For initial data $\varphi \in \mathscr{H}_0$, the first component $u(x, t) = (W_0(t)\varphi)_1$ satisfies the free wave equation (186) if φ is smooth enough. The primary fact that we need is Huygens' principle:

Theorem XI.87 (Huygens' principle) Let $W_0(t)$ be the unitary group for the free wave equation on $\mathbb{R}^3$ and set $u(x, t) = (W_0(t)\varphi)_1$. Suppose that $\varphi = \langle f, g\rangle \in \mathscr{H}$ has compact support. Then

$$\operatorname{supp} u(x, t) \subset \left\{x \,\middle|\, |x - y| = t \text{ for some } y \in \operatorname{supp}\langle f, g\rangle\right\}$$

Proof Suppose first that $f = 0$ and that $g \in C_0^\infty(\mathbb{R}^3)$. We shall derive an explicit formula for the solution of (186) in the case $c_0 = \rho_0 = 1$. In order to solve (186), we need just find a u so that $\hat{u}_{tt}(k, t) = -k^2\hat{u}(k, t)$, $\hat{u}(k, 0) = 0$, and $\hat{u}_t(k, 0) = \hat{g}(k)$. This is easily done by setting

$$\hat{u}(k, t) = \frac{\sin|k|t}{|k|}\hat{g}(k)$$

Let H be the tempered distribution whose Fourier transform is $|k|^{-1}\sin|k|t$. Then

$$\begin{aligned}u(x, t) &= \mathscr{F}^{-1}(|k|^{-1}\sin|k|t\hat{g}(k)) \\ &= (2\pi)^{-3/2}H * g\end{aligned}$$

so in order to represent the solution we must just find H. Let dS_R denote the area measure on the sphere of radius R. dS_R is a tempered distribution and using θ for the angle between x and k,

$$\begin{aligned}\widehat{dS_R}(k) &= (2\pi)^{-3/2}\int e^{-ik\cdot x}\,dS_R(x)\\ &= (2\pi)^{-3/2}\int_0^{\pi} d\theta \int_0^{2\pi} e^{-i|k|R\cos\theta} R^2 \sin\theta\, d\psi\\ &= (2\pi)^{-1/2} R^2 \int_0^{\pi} e^{-i|k|R\cos\theta}\sin\theta\, d\theta\\ &= \frac{2R\sin|k|R}{(2\pi)^{1/2}|k|}\end{aligned}$$

Thus for $t > 0$, $H = (2t)^{-1}(2\pi)^{1/2}\,dS_t$ and

$$u(x,t) = \frac{1}{4\pi t}\int_{\mathbb{R}^3} g(x+y)\,dS_t(y)$$

A similar representation holds for $t < 0$. Notice that $v = u_t$ satisfies (186) too, along with the initial conditions $v(0,t) = g$, $v_t(0,t) = 0$. Thus, for $f, g \in C_0^\infty(\mathbb{R}^3)$, we can write the solution of (186) as

$$u(x,t) = \frac{1}{4\pi t}\int_{\mathbb{R}^3} g(x+y)\,dS_t(y) + \frac{d}{dt}\left(\frac{1}{4\pi t}\int_{\mathbb{R}^3} f(x+y)\,dS_t(y)\right) \quad (216a)$$

and from this representation Huygens' principle follows immediately for C_0^∞ data.

Now suppose that $\varphi = \langle f, g\rangle \in \mathscr{H}_0$ with support in a compact set K and let Σ_t be the set where $u(x,t)$ is supposed to be supported according to Huygens' principle. Let $K^{(\varepsilon)}$ and $\Sigma_t^{(\varepsilon)}$ be the sets K and Σ_t plus all the points a distance less than ε away. Then there is a sequence $\varphi_n = \langle f_n, g_n\rangle$ of pairs of C_0^∞ functions with support in $K^{(\varepsilon)}$ so that $\varphi_n \to \varphi$ in $\mathscr{H}_0$. Since $W_0(t)$ is unitary, $W_0(t)\varphi_n \to W_0(t)\varphi$ and, in particular,

$$\int_{\mathbb{R}^3} |\nabla(u_n - u)(x)|^2\,dx \to 0$$

By the uncertainty principle lemma (Section X.2),

$$\begin{aligned}\int_{|x|\le r} |u(x,t) - u_n(x,t)|^2\,dx &\le 4r^2\int_{\mathbb{R}^3}\frac{1}{4|x|^2}|u(x,t) - u_n(x,t)|^2\,dx\\ &\le 4r^2\int_{\mathbb{R}^3}|\nabla(u(x,t) - u_n(x,t))|^2\,dx \qquad (216b)\end{aligned}$$

so that in each ball of radius r a subsequence of $\{u_n\}$ converges to u pointwise a.e. Thus u is zero outside $\Sigma^{(\varepsilon)}$ since each of the u_n is zero there. Since ε is arbitrary, u is supported in Σ_t. ∎

Corollary Suppose that $\operatorname{supp}\langle f, g\rangle$ is contained in the ball of radius r. Then

$$u(x,t) = 0 \quad \text{for} \quad |x| > r + t \qquad (217a)$$

$$u(x,t) = 0 \quad \text{for} \quad |x| < |t| - r \qquad (217b)$$

(217a) is an expression of the finite propagation speed and holds in all dimensions. (217b) is an expression of Huygens' principle which holds only in odd dimensions greater than or equal to three.

Now we define

$$D_+ = \{\varphi \in \mathscr{H}_0 \,|\, u(x,t) = (W_0(t)\varphi)_1 \text{ is zero for } |x| \le t,\ t > 0\}$$

$$D_- = \{\varphi \in \mathscr{H}_0 \,|\, u(x,t) = (W_0(t)\varphi)_1 \text{ is zero for } |x| \le -t,\ t < 0\}$$

To check that D_+ is an outgoing subspace we proceed as follows. D_+ is closed by the unitarity of $W_0(t)$ and the inequality (216b). To prove (i) notice that if $\varphi \in D_+$, then

$$(W_0(t)W_0(s)\varphi)_1 = (W_0(t+s)\varphi)_1 = u(x, t+s)$$

so $(W_0(t)W_0(s)\varphi)_1$ is zero if $t > 0$ and $|x| \le t + s$. Thus if $s \ge 0$, $W_0(s)\varphi \in D_+$. Secondly, suppose that $\psi \in \bigcap_s W_0(s)[D_+]$. Since $\varphi \in D_+$ implies that

$$\operatorname{supp}(W_0(s)\varphi)_1 \subset \mathbb{R}^3 \setminus \left\{x \,\middle|\, |x| \le s\right\}$$

$\psi \in W_0(s)[D_+]$ for all $s > 0$ implies that $(\psi)_1 \equiv 0$. But for $\varphi \in D_+$, $(d/dt) \times (W_0(t)\varphi)_1 = (W_0(t)\varphi)_2$ so $(\psi)_2 \equiv 0$ too. Thus $\psi \equiv 0$, which proves (ii). Finally, notice that if $\operatorname{supp}\varphi \subset \{x \,|\, |x| \le R\}$, then by (217b), $W_0(R)\varphi \in D_+$. Thus, $\bigcup_t W_0(t)D_+$ contains all the C^∞ data of compact support, so (iii) holds. The proof that D_- is incoming is similar. Thus by Theorem XI.82 there exist incoming and outgoing translation representations for $W_0(t)$.

In practice one wants a translation representation that is both incoming *and* outgoing for $W_0(t)$ and lots of detailed information, and therefore one constructs the representation directly instead of appealing to Theorem XI.82. The construction is accomplished by noticing that for each $\sigma \in \mathbb{R}$ and $\omega \in \mathbb{R}^3$ with $|\omega| = 1$,

$$\varphi_{\sigma,\omega} = e^{-i\sigma\omega\cdot x}\begin{pmatrix}1\\ -i\sigma\end{pmatrix}$$

is an (improper) eigenfunction of

$$A_0 = i\begin{pmatrix} 0 & I \\ \Delta & 0 \end{pmatrix}$$

with eigenvalue $+\sigma$. Analogously to Section 6, we now define

$$f^*(\sigma, \omega) = (2\pi)^{-3/2}(f, \varphi_{\sigma,\omega})_{\mathscr{H}_0}$$

for $f \in C_0^\infty(\mathbb{R}^3) \times C_0^\infty(\mathbb{R}^3)$. We can regard f^* as a function on $\mathbb{R}$ with values in $N = L^2(S^2)$, and it is not hard to show that the map $f \to f^*$ is an isometry of $\mathscr{H}_0$ into $L^2(\mathbb{R}; L^2(S^2))$. In fact the map is unitary and since

$$(A_0 f)^*(\sigma, \omega) = (A_0 f, \varphi_{\sigma,\omega}) = (f, A_0\varphi_{\sigma,\omega}) = \sigma(f, \varphi_{\sigma,\omega}) = \sigma f^*(\sigma, \omega)$$

A_0 goes over to multiplication by σ. Taking the inverse Fourier transform in the σ variables, one obtains a representation of $\mathscr{H}_0$ as $L^2(\mathbb{R}; L^2(S^2))$ in which $W_0(t)$ is represented as right translation. What is not obvious in this construction is what happens to D_+ and D_-. But it can be shown explicitly that D_+ and D_- go over to $L^2(0, \infty, S^2)$ and $L^2(-\infty, 0; S^2)$, respectively. This shows that the translation representation is both incoming *and* outgoing and, incidentally, that $\mathscr{H}_0 = D_+ \oplus D_-$, a fact that is certainly not obvious in the original representation. This orthogonality gives rise to some of the analyticity properties of the scattering operator which we shall discuss below.

Finally, we remark that the explicit construction of the translation representation can itself be used to provide a proof of Huygens' principle.

Example 2 (acoustic waves in an inhomogeneous medium) Let us consider the first example, (187), of the preceding section from the Lax–Phillips point of view:

$$u_{tt} = c(x)^2\rho(x)\nabla \cdot \frac{1}{\rho(x)}\nabla u$$

$$u(x, 0) = f(x), \qquad u_t(x, 0) = g(x)$$

We assume all the hypotheses on $c(x)$, $\rho(x)$ that we made in Section 10 and use without comment the spaces and operators H_1, $L^2_{\rho c}(\mathbb{R}^3)$, $\mathscr{H}_1$, B_1, A_1, $W_1(t)$ constructed there. We make one additional assumption on $c(x)$ and $\rho(x)$, namely

$$\rho(x) \equiv 1, \qquad c(x) \equiv 1, \qquad |x| \geq r$$

for some r.

Now, let $r_0 > r$ and let D_+ and D_- be defined as in Example 1. We set

$$D_+^{r_0} \equiv W_0(r_0)D_+, \qquad D_-^{r_0} \equiv W_0(-r_0)D_-$$

Notice that $D_+^{r_0}$, $D_-^{r_0}$ are closed subspaces of $\mathscr{H}_0$. They are also closed subspaces of $\mathscr{H}_1$ since $\varphi \in D_\pm^{r_0}$ implies that φ vanishes inside the ball $B(r_0)$, of radius r_0, so

$$\|\varphi\|_{\mathscr{H}_1} = \|\varphi\|_{\mathscr{H}_0}, \qquad \varphi \in D_\pm^{r_0}$$

since the norms are the same for functions with support outside $B(r)$. We choose J to be the identity operator.

Suppose that $\varphi \in C_0^\infty(\mathbb{R}^3) \times C_0^\infty(\mathbb{R}^3)$ and that $\varphi \in D_+^{r_0}$. Since $W_0(t)$: $D_+^{r_0} \to D_+^{r_0}$ for $t \geq 0$, we have

$$(W_0(t)\varphi)' = -iA_0 W_0(t)\varphi = -iA_1 W_0(t)\varphi$$

because A_0 and A_1 coincide on smooth functions with support outside $B(r)$. By the uniqueness of semigroups, $W_0(t)\varphi = W_1(t)\varphi$ for $t \geq 0$ and since such φ are dense in $D_+^{r_0}$, we have

$$W_1(t)\varphi = W_0(t)\varphi, \qquad \varphi \in D_+^{r_0}, \quad t \geq 0 \tag{218}$$

and similarly

$$W_1(t)\varphi = W_0(t)\varphi, \qquad \varphi \in D_-^{r_0}, \quad t \leq 0$$

This shows that W_0 and W_1 satisfy hypotheses (0) and (2) of Theorem XI.86. That condition (3) holds is just what we sketched in Example 1. Further, we know that $D_-^{r_0}$ and $D_+^{r_0}$ are incoming and outgoing subspaces for $W_0(t)$. What we need to show is that they are also incoming and outgoing for $W_1(t)$. By Theorem XI.82, the Lax–Phillips scattering operator $\tilde{S}$ will then exist. And, since hypotheses (0)–(3) of Theorem XI.86 hold, we shall have a new proof that the wave operators exist and are complete, and $(\Omega^-)^{-1}\Omega^+$ will be related to $\tilde{S}$ by (215).

To show that $D_+^{r_0}$ is outgoing for $W_1(t)$, we must verify (i)–(iii). Properties (i) and (ii) follow immediately form (215) and the corresponding statements for the free group proved in Example 1. Property (iii) is much harder and uses a whole array of technical tools. Besides Huygens' principle we shall need a compact embedding theorem of the type discussed in Section XIII.14 and a detailed spectral analysis of A_1. Our plan is to show that (iii) is equivalent to a form of energy decay in the neighborhood of the inhomogeneity and then to prove the energy decay using properties of A_1. Since (iii) implies asymptotic completeness, it is not surprising that it is related to an energy decay condition: We expect asymptotic completeness to hold only if any solution of the interacting equation looks free in the distant future and distant part, that is, if it propagates away from the region of inhomogeneity.

We begin with a lemma which shows that for the free equation, energy propagates at speed one. For any $R > 0$ and $\varphi = \langle u, v \rangle$, define the local energy norms as follows:

$$\|\varphi\|_0^{(R)} \equiv \int_{|x| \le R} |\nabla u|^2 + |v|^2 \, dx$$

$$\|\varphi\|_1^{(R)} \equiv \int_{|x| \le R} \rho(x)^{-1} |\nabla u|^2 + (c(x)^2 \rho(x))^{-1} |v|^2 \, dx$$

Lemma 1

(a) For any $R > 0$,

$$\|W_0(T)\varphi\|_0^{(R)} \le \|\varphi\|_0^{(R+T)} \qquad \text{for all} \quad \varphi \in \mathscr{H}_0$$

(b) For any $R \ge r_0$,

$$\|W_1(T)\varphi\|_1^{(R)} \le \|\varphi\|_1^{(R+T)} \qquad \text{for all} \quad \varphi \in \mathscr{H}_1$$

Proof The idea is to integrate an "energy flux" over the surface of the region $\Omega(R, T)$ given by $|x| \le R + T - t$, $0 \le t \le T$, shown in Figure XI.14. Because of conservation of energy, no net flux can be produced inside

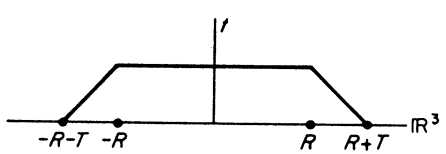


FIGURE XI.14 $\Omega(R, T)$.

$\Omega(R, T)$, and because of the finite propagation speed, flux can flow only out of the sides; so the flux in at the bottom $\|\cdot\|_i^{(R+T)}$ must be greater than the flux out at the top $\|W_i(T)\cdot\|_i^{(R)}$.

Explicitly, define

$$j_0(x, t) = \tfrac{1}{2}[(c^2(x)\rho(x))^{-1} |u_t(x, t)|^2 + \rho(x)^{-1} |\nabla u(x, t)|^2]$$

$$j_i(x, t) = -\rho(x)^{-1} \operatorname{Re}\{\overline{u_t}(x, t)\, \partial_i u(x, t)\}$$

and set $j = \langle j_0, \mathbf{j} \rangle$. We will see in the appendix to Section 13 that these are four of the components of the energy-momentum tensor. Suppose first that $\varphi = \langle f, g \rangle$ with $f, g \in C_0^\infty$. Let $u(x, t) = (W_1(t)\varphi)_1$. Standard arguments of

the type used in Section X.13 show that u is C^∞ in x and t. A direct calculation using $u_{tt} = c^2\rho\nabla \cdot \rho^{-1}\nabla u$ shows that

$$\nabla_{\mathbb{R}^4} \cdot j = \frac{\partial j_0}{\partial t} + \sum_{i=1}^{3} \frac{\partial j_i}{\partial x_i} = 0$$

So, by Gauss's theorem,

$$\int_{\partial\Omega(R, T)} j \cdot \sigma \, dS = 0$$

where $\sigma = \langle \sigma_0, \boldsymbol{\sigma} \rangle$ is the outward pointing normal and dS is the surface measure. By the inequality $2ab \le a^2 + b^2$, $|\mathbf{j}(x, t)| \le j_0(x, t)$ at points where $c = 1$, such as the sides of Ω. Moreover, $|\boldsymbol{\sigma}(x, t)| = \sigma_0(x, t)$ on the sides of Ω. It follows that $j \cdot \sigma \ge 0$ on the sides of Ω so

$$\int_{|x| \le R} j_0(x, T) \, dx \le \int_{|x| \le R+T} j_0(x, 0) \, dx$$

which proves (b) for smooth φ. A limiting argument proves (b) for all $\varphi \in \mathscr{H}_1$. A similar argument proves (a). ∎

With this lemma, we can now show that (iii) is equivalent to a weak form of local energy decay.

Lemma 2 Under the hypotheses in Example 2, (iii) holds if and only if

$$\lim_{t \to +\infty} \|W_1(t)\varphi\|_1^{(R)} = 0 \tag{219}$$

for all $\varphi \in \mathscr{H}_1$ and all $R < \infty$.

Proof First, suppose that (iii) holds. Then, given any $\varphi \in \mathscr{H}_1$ and $\varepsilon > 0$, there is a t_0 and a $\psi \in D_+^{r_0}$ so that $\|W_1(t_0)\psi - \varphi\|_1 \le \varepsilon$. Now, since $\psi \in D_+^{r_0}$, $W_1(t + t_0)\psi$ vanishes in $B(R)$ if $t > R - t_0$. Thus since

$$\|W_1(t)\varphi - W_1(t + t_0)\psi\|_1 = \|\varphi - W_1(t_0)\psi\|_1 \le \varepsilon$$

for all t, we have

$$\|W_1(t)\varphi\|_1^{(R)} \le \varepsilon \qquad \text{for} \quad t \ge R - t_0$$

Therefore $\lim_{t\to\infty} \|W_1(t)\varphi\|_1^{(R)} = 0$, which is a priori stronger than (219).

To prove the converse, suppose that (219) holds and that ψ is perpendicular to $\overline{\bigcup W_1(t)D_+^{r_0}}$, which is the same as saying that $W_1(t)\psi \perp D_+^{r_0}$ for all t. From the fact that the free translation representation of $D_+^{r_0}$ is all of

$L^2(r_0, \infty; N)$, we conclude that $W_0(-2r_0)W_1(t)\psi \in D^{r_0}_-$ for all t. Since $W_1(-s)$ and $W_0(-s)$ agree on $D^{r_0}_-$ for $s \geq 0$, we have

$$W_0(-(s+2r_0))W_1(t)\psi = W_1(-s)W_0(-2r_0)W_1(t)\psi \tag{220}$$

and also that $W_0(-s)W_1(t)\psi$ is zero for $|x| < s - r_0$.

Now, given $\varepsilon > 0$, by (219) we can find a $t > (k+1)r_0$ such that

$$\|W_1(t)\psi\|_1^{(5r_0)} < \varepsilon$$

so by Lemma 1,

$$\|W_0(-2r_0)W_1(t)\psi\|_1^{(3r_0)} \leq d\|W_0(-2r_0)W_1(t)\psi\|_0^{(3r_0)} \leq d_0\varepsilon$$
$$\|W_1(t-2r_0)\psi\|_1^{(3r_0)} \leq \varepsilon$$

where d_0 is a universal constant relating the two equivalent norms $\|\cdot\|_1$ and $\|\cdot\|_0$. Notice that $W_0(-s)W_1(t)\psi = W_1(-s)W_1(t)\psi$ at $s = 0$, and thus these two solutions will be equal for $|x| > |s| + r_0$ since the solution at such points is not affected by the inhomogeneity inside $B(r_0)$. In particular,

$$(W_0(-2r_0)W_1(t)\psi)(x) = (W_1(-2r_0)W_1(t)\psi)(x)$$

for $|x| > 3r_0$. This fact and the estimates above imply that

$$\|W_0(-2r_0)W_1(t)\psi - W_1(t-2r_0)\psi\|_1 \leq (1+d_0)\varepsilon$$

Now set $s = t - 2r_0$. Since $W_1(2r_0 - t)$ is unitary, we have (using (220))

$$\|W_0(-t)W_1(t)\psi - \psi\|_1 \leq (1+d_0)\varepsilon$$

But recall that $W_0(-t)W_1(t)\psi$ is zero for $|x| < t - r_0$. Choosing $t > (k+1)r_0$, we have that

$$\|\psi\|_1^{(kr_0)} \leq (1+d_0)\varepsilon$$

Since ε and k are arbitrary, we conclude that $\psi = 0$. Thus (iii) holds. ∎

To prove (219), we need a local compactness result.

Lemma 3 Fix c_1. The set $\mathscr{K}$ of $\varphi \in D(A_1)$ such that $\|A_1\varphi\|_1 + \|\varphi\|_1 \leq c_1$ is compact in the $\|\cdot\|_1^{(R)}$-norm for each R; that is, given any sequence in $\mathscr{K}$, there is a subsequence converging in the $\|\cdot\|_1^{(R)}$-norm.

Proof Let $\varphi = \langle u, v\rangle$. The condition of the hypothesis says that

$$\|B_1^2 u\|_{\rho c}^2 + \|B_1 u\|_{\rho c}^2 + \|B_1 v\|_{\rho c}^2 + \|v\|_{\rho c}^2 \leq c_1$$

for some c_1. Using the conditions (190) on c and ρ, one easily obtains from this that

$$\|\Delta u\|_2^2 + \|\nabla u\|_2^2 + \|\nabla v\|_2^2 + \|v\|_2^2 \leq c_2$$

for all φ in the original set $\mathscr{K}$. By Corollary 1 to Theorem XIII.74, the set of $v \in L^2$ satisfying $\|\nabla v\|_2^2 + \|v\|_2^2 \leq c_2$ is compact in the local norm $\|v\|_2^{(R)}$; and similarly, the set satisfying $\|\Delta u\|_2^2 + \|\nabla u\|_2^2 \leq c_2$ is compact in the local norm $\|\nabla u\|_2^{(R)}$. Thus $\mathscr{K}$ is compact in the local norm $\|\cdot\|_0^{(R)}$, and therefore also in $\|\cdot\|_1^{(R)}$ since the norms are equivalent. ∎

Finally, we need spectral information on A_1.

Lemma 4 A_1 has purely absolutely continuous spectrum.

Proof This will clearly be true if $B_1^2 = -c(x)^2\rho(x)\nabla\cdot\rho(x)^{-1}\nabla$ has purely absolutely continuous spectrum on $L^2_{\rho c}(\mathbb{R}^3)$. B_1^2 is unitarily equivalent to the operator

$$\tilde{B}_1^2 = -(c(x)^2\rho(x))^{1/2} \circ \nabla\cdot\rho(x)^{-1}\nabla \circ (c(x)^2\rho(x))^{1/2}$$

on $L^2(\mathbb{R}^3)$. In Theorem XIII.62 we shall show that such an operator has no eigenvalues. In Theorem XI.45 we showed that matrix elements of the resolvent are bounded for a dense set of vectors as one approaches the real axis. This fact implies that there is no singular continuous spectrum (Theorem XIII.19). ∎

We are now ready to complete the argument and prove (iii). Let φ be in $D(A_1)$ and consider the set $\mathscr{K}_\varphi = \{U_1(t)\varphi \mid t \in \mathbb{R}\}$. Since

$$\|A_1 U_1(t)\varphi\|_1 + \|U_1(t)\varphi\|_1 = \|A_1\varphi\|_1 + \|\varphi\|_1$$

$\mathscr{K}_\varphi$ is compact in $\|\cdot\|_1^{(R)}$ by Lemma 3. Moreover, A_1 has purely absolutely continuous spectrum, so $(U_1(t)\varphi, \psi)_1 \to 0$ as $t \to +\infty$ for all φ, ψ by the Riemann–Lebesgue lemma. It follows that any $\|\cdot\|_1^{(R)}$ limit point must be zero, so, by the compactness,

$$\lim_{t\to+\infty} \|U_1(t)\varphi\|_1^{(R)} = 0$$

Since $D(A_1)$ is dense in $\mathscr{H}_1$ and $U_1(t)$ is unitary, this holds for all $\varphi \in \mathscr{H}_1$ and all $R > 0$ which, by Lemma 2, proves (iii). We summarize:

Theorem XI.88 Let $c(x)$ and $\rho(x)$ be smooth functions that equal constants outside of a compact set and satisfy (190). Then $D^{r_0}_+$ and $D^{r_0}_-$ are outgoing and incoming subspaces for $W_1(t) = e^{-iA_1 t}$ on $\mathscr{H}_1$, so by Theorem XI.82, the Lax–Phillips scattering operator exists. Further, for any identification operator $J: \mathscr{H}_0 \to \mathscr{H}_1$ which is the identity on $D^{r_0}_\pm$, the wave operators $\Omega^\pm(A_0, A_1, J)$ exist, are complete, and are related to the Lax–Phillips scattering operator by the formula (215).

It is worthwhile to point out here an important difference between the Lax–Phillips approach and that of Section 10. In order to construct the Lax–Phillips scattering operator, we needed the fact that A_1 has purely absolutely continuous spectrum; actually, with a longer argument (the RAGE theorem), purely continuous spectrum is enough. Except for constant coefficient operators where one can use the Fourier transform, the elimination of point spectrum is a hard problem (see Theorem XIII.62). Thus the Lax–Phillips approach requires quite delicate information about the generator of the interacting dynamics. This information is not required for the approach of Section 10, which uses the Kato–Birman theory. Of course, the conclusion we got there was weaker in that we knew only that $\operatorname{Ran}\Omega^+ = \mathscr{H}_{ac}(A_1) = \operatorname{Ran}\Omega^-$, and not $\mathscr{H}_{ac}(A_1) = \mathscr{H}_1$. But $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^-$ is all that one needs to construct the scattering operator itself.

We now return to the abstract theory and investigate properties of the scattering operators $\tilde{S}$ and $\hat{S} = \mathscr{F}\tilde{S}\mathscr{F}^{-1}$ on $L^2(\mathbb{R}; N)$.

Proposition Let D_+ and D_- be outgoing and incoming subspaces for a unitary group $U(t)$ on $\mathscr{H}$. Then:

(a) The scattering operator $\tilde{S}$ on $L^2(\mathbb{R}; N)$ commutes with translation.
(b) If D_+ and D_- are orthogonal to each other, then

$$\tilde{S}\colon L^2(-\infty, 0; N) \to L^2(-\infty, 0; N)$$

Proof Let $\mathscr{R}_\pm$ be the maps onto the outgoing and incoming translation representations of $\mathscr{H}$, $U(t)$, $D^\pm$. Then

$$\tilde{S}T_0(s) = \mathscr{R}_+\mathscr{R}_-^{-1}T_0(s) = \mathscr{R}_+ U(s)\mathscr{R}_-^{-1} = T_0(s)\mathscr{R}_+\mathscr{R}_-^{-1} = T_0(s)\tilde{S}$$

where $T_0(s)$ is translation by s units. This proves (a). (b) is also easy. For if $f \in L^2(-\infty, 0; N)$, then $\mathscr{R}_-^{-1}f \in D_-$ and since D_- is orthogonal to D_+ we know that $\tilde{S}f = \mathscr{R}_+\mathscr{R}_-^{-1}f$ is orthogonal to $\mathscr{R}_+ D_+$. But, $\mathscr{R}_+ D_+ \equiv L^2(0, \infty; N)$, so $\tilde{S}f \in L^2(-\infty, 0; N)$. ∎

As we have already noted, if (0)–(3) hold, then D_+^{r0} and D_-^{r0} are *orthogonal* outgoing and incoming subspaces for $U(t)$. Some analyticity of $\hat{S}$ follows from the following general theorem.

Theorem XI.89 Let N be a separable Hilbert space and T a bounded operator on $L^2(\mathbb{R}; N)$ such that T commutes with translation and takes $L^2(-\infty, 0; N)$ into itself. Then, $\hat{T} = \mathscr{F}T\mathscr{F}^{-1}$ operates on $L^2(\mathbb{R}; N)$ by multiplication by an $\mathscr{L}(N)$-valued function $t(\sigma)$:

$$(\hat{T}f)(\sigma) = t(\sigma)f(\sigma) \tag{221}$$

Further, there is a norm analytic $\mathscr{L}(N)$-valued function $t(\sigma + iy)$ in the open upper half-plane so that:

(a) $\|t(\sigma + iy)\|_{\mathscr{L}(N)} \le \|T\|$, $\sigma \in \mathbb{R}$, $y > 0$;
(b) $t(\sigma + iy)$ converges weakly to $t(\sigma)$ for almost all $\sigma \in \mathbb{R}$ as $y \downarrow 0$.

Proof We consider first the case where $N = \mathbb{C}$. Suppose that T is an operator on $L^2(\mathbb{R}; \mathbb{C})$ that commutes with translations. We first claim that (221) holds. Given (221), it is clear that $t \in L^\infty$ and $\|t\|_\infty = \|\hat{T}\| = \|T\|$.

There are two different ways of proving (221). First note that T is a linear map of $\mathscr{S}(\mathbb{R})$ into $L^2(\mathbb{R})$. Since T commutes with translations, it is easy to check that T is actually a continuous map of $\mathscr{S}(\mathbb{R})$ into $C^\infty(\mathbb{R})$. Thus, by Problem 9 of Chapter IX, there is a distribution $\tau \in \mathscr{S}'$ such that

$$T(f) = \tau * f$$

for $f \in \mathscr{S}(\mathbb{R})$. Thus there is a distribution $t \in \mathscr{S}'$ such that (221) holds for $f \in \mathscr{S}$. Since

$$\left|\int \overline{g(\sigma)}t(\sigma)f(\sigma)\,d\sigma\right| = |(g, \hat{T}f)| \le \|\hat{T}\|\,\|g\|_2\|f\|_2$$

we conclude that t is a bounded function and (221) holds for all $f \in L^2(\mathbb{R})$. The second proof argues that since T commutes with translation, $\hat{T}$ commutes with multiplication by e^{ita} for all a. By a limiting argument, $\hat{T}$ commutes with multiplication by any bounded measurable function. (221) then follows immediately from Theorem XIII.84.

The first step in proving the analyticity is to show that τ has support on $(-\infty, 0]$. Let j be a positive function in $C_0^\infty(-\infty, 0)$ with $\int j(x)\,dx = 1$ and define $j_\delta(x) = \delta^{-1}j(x/\delta)$, $\tau_\delta = \tau * j_\delta$. Then

$$f \mapsto \tau_\delta * f = T(j_\delta * f)$$

takes $L^2(-\infty, 0)$ to itself. If we can show that each τ_δ has support in $(-\infty, 0]$, then so does τ since $\tau_\delta \to \tau$. Thus, it suffices to prove the support property in the case where τ is a C^∞ function. Suppose that $\tau(a) \neq 0$ for some $a > 0$. Then we can find δ and θ so that $\operatorname{Re}(e^{i\theta}\tau(x)) > 0$ for all $x \in (a - \delta, a + \delta)$. Letting f be the characteristic function of $(-\delta, 0)$, we see that $\operatorname{Re}\{e^{i\theta}(\tau * f)(x)\} > 0$ for $x \in (a, a + \delta)$, which violates the hypothesis that T leaves $L^2(-\infty, 0)$ invariant. Thus τ has support on $(-\infty, 0]$.

Since τ has support on the half-line, Theorem IX.16 implies that t is the boundary value in the sense of distributions of an analytic function $t(\sigma + iy)$ in the upper half-plane satisfying

$$|t(\sigma + iy)| \le C(1 + \sigma^2 + y^2)^{N_1}(1 + y^{-N_2})$$

for some C, N_1, and N_2. We want to show that t is bounded in the upper half-plane with $\|t\|_\infty \le \|T\|$. Let $\tau_\varepsilon(x) = (2\pi)^{1/2} e^{-\varepsilon x^2}\tau(x)$ and define

$$t_\varepsilon(\sigma + iy) \equiv (2\pi)^{-1/2} \int \tau_\varepsilon(x) e^{-i(\sigma+iy)x}\, dx$$

$$= \int t(\sigma + iy - \mu) \frac{e^{-\mu^2/4\varepsilon}}{\sqrt{4\pi\varepsilon}}\, d\mu$$

Then, for fixed $y > 0$, $t_\varepsilon(\cdot + iy) \to t(\cdot + iy)$ pointwise, so it suffices to show that $\|t_\varepsilon(\cdot + iy)\|_\infty \le \|T\|$ for each ε and y. Now, since τ is tempered, it is the Nth derivative of a polynomially bounded continuous function h. It follows that t_ε is entire and

$$|t_\varepsilon(\sigma + iy)| = \int |[D^N h](e^{-\varepsilon x^2} e^{-i(\sigma+iy)x})|\, dx$$

$$\le C(1 + |\sigma + iy|)^N$$

Let $\delta > 0$ be a given small number, and define

$$t_{\varepsilon,\delta}(\sigma + iy) = (1 - i\delta(\sigma + iy))^{-N} t_\varepsilon(\sigma + iy)$$

If $Y \ge 2\delta^{-1} + 1$, then

$$\frac{1 + |\sigma + iY|}{|1 - i\delta(\sigma + iY)|} \le \frac{2}{\delta}$$

for all σ, so

$$\|t_{\varepsilon,\delta}(\cdot + iY)\|_\infty \le C\left(\frac{2}{\delta}\right)^N$$

and

$$\|t_{\varepsilon,\delta}(\cdot + i0)\|_\infty \le \|t_\varepsilon(\cdot + i0)\|_\infty \le \|T\|$$

Since $t_{\varepsilon,\delta}$ is bounded, Hadamard's three lines theorem implies that

$$\|t_{\varepsilon,\delta}(\cdot + iy)\|_\infty \le \|T\|^{1-y/Y} \left[C\left(\frac{2}{\delta}\right)^N\right]^{y/Y}$$

for each y satisfying $0 < y < Y$. Holding y fixed and taking Y to infinity, we see that

$$\|t_{\varepsilon,\delta}(\cdot + iy)\|_\infty \le \|T\|$$

Finally, letting $\delta \to 0$ and then $\varepsilon \to 0$, we conclude that $\|t(\cdot + iy)\|_\infty \le \|T\|$ for each $y > 0$.

Continuity at the real axis follows from a general complex variables result which we state after the theorem.

Now let N be an arbitrary Hilbert space. For $\varphi, \eta \in N$,

$$T_{\varphi,\eta}: f \to (\varphi, T(f\eta))_N$$

maps $L^2(\mathbb{R})$ into itself and $L^2(-\infty, 0)$ into itself. So, by the scalar case,

$$\widehat{T_{\varphi,\eta}(f)} = t_{\varphi,\eta}(\sigma) f(\sigma)$$

where $t_{\varphi,\eta}(\sigma + iy)$ is analytic in the upper half-plane, has $t_{\varphi,\eta}(\sigma)$ as boundary value, and satisfies

$$|t_{\varphi,\eta}(\sigma + iy)| \le \|T_{\varphi,\eta}\| \le \|T\|\, \|\varphi\|_N\, \|\eta\|_N$$

in the closed upper half-plane. Since $\langle \varphi, \eta \rangle \to T_{\varphi,\eta}$ is sesquilinear, so is $\langle \varphi, \eta \rangle \to t_{\varphi,\eta}(\sigma + iy)$ for each σ and $y \ge 0$. Thus, by the Riesz lemma, for each $\sigma + iy$, there is a bounded operator $t(\sigma + iy)$ on N so that

$$t_{\varphi,\eta}(\sigma + iy) = (\varphi, t(\sigma + iy)\eta)_N$$

$t(\sigma + iy)$ is clearly weakly analytic and multiplication by $t(\sigma)$ on $L^2(\mathbb{R}; N)$ is $\mathscr{F}T\mathscr{F}^{-1}$. Norm analyticity follows from the fact that $\|t(\sigma + iy)\|$ is uniformly bounded and the methods of Theorem VI.4 (Problem 123). Since $t_{\varphi,\eta}(\sigma + iy)$ has $t_{\varphi,\eta}(\sigma)$ as its pointwise limit as $y \downarrow 0$ for almost all σ, $t(\sigma + iy)$ has $t(\sigma)$ as its limit in the weak operator topology on N for almost all σ. ∎

In the above proof, continuity up to the axis follows from the following result (see the reference in the Notes):

Lemma (Fatou's theorem) If $F(z)$ is analytic in the upper half-plane and

$$\sup_{y>0} \int |F(x + iy)|^p\, dx < \infty$$

for some $p > 1$ (where $p = \infty$ is allowed), then for almost all $x \in \mathbb{R}$,

$$\lim_{y \downarrow 0} F(x + iy) \equiv f(x)$$

exists, $f \in L^p$, and $F(\cdot + iy) \to f(\cdot)$ in the sense of distributions.

Applying Theorem XI.89 to the case we are interested in, we have:

Corollary Suppose that there exist orthogonal incoming and outgoing subspaces for a unitary group $U(t)$ on a Hilbert space $\mathscr{H}$. Then, there is an $\mathscr{L}(N)$-valued function $s(\sigma + iy)$ on the closed upper half-plane satisfying:

(1) $s(\sigma + i0)$ is unitary almost everywhere.
(2) $s(\sigma + iy)$ is norm analytic in the open upper half-plane with

$$\|s(\sigma + iy)\|_{\mathscr{L}(N)} \leq 1$$

(3) $s(\sigma + iy)$ converges strongly to $s(\sigma)$ almost everywhere as $y \downarrow 0$ and, for all $f \in L^2(\mathbb{R}; N)$,

$$(\hat{S}f)(\sigma) = s(\sigma)f(\sigma)$$

and $\hat{S}$ takes $\mathscr{H}^2_+(\mathbb{R}; N)$ into itself.

Proof All the statements of the theorem except *strong* continuity up to the real axis follow immediately from Theorem XI.89 and the previous proposition. Strong continuity follows from weak continuity since

$$\begin{aligned}\|s(\sigma + iy)\varphi - s(\sigma)\varphi\|_N^2 &= \|s(\sigma + iy)\varphi\|_N^2 - (s(\sigma + iy)\varphi, s(\sigma)\varphi)_N \\ &\quad - (s(\sigma)\varphi, s(\sigma + iy)\varphi)_N + \|s(\sigma)\varphi\|_N^2 \\ &\to 0\end{aligned}$$

because $\|s(\sigma + iy)\| \leq 1 = \|s(\sigma)\|$. ∎

As in the quantum-mechanical case discussed in Section 7, the analytic continuation properties of the scattering operator are important. Thus one wants general methods for investigating the continuation properties of $s(z)$. Since $s(z)$ is unitary on the real axis, the natural way to try to continue it to the lower half-plane is by the formula

$$s(z) = [s(\bar{z})^*]^{-1}, \qquad \operatorname{Im} z < 0$$

But for this formula to work we need to know that zero is in the resolvent set of $s(\bar{z})$, that is, that $s(\bar{z})$ is *regular*. In order to do this, Lax and Phillips introduced the following semigroup:

Let $\mathscr{K} = (D_+ \oplus D_-)^\perp$ and let $P_\mathscr{K}$ be the orthogonal projection onto $\mathscr{K}$. Define

$$Z(t) = P_\mathscr{K} U(t) P_\mathscr{K}, \qquad t \geq 0 \tag{222}$$

$Z(t)$ is clearly the restriction of the dynamics to the states that are neither incoming in the past nor outgoing in the future, so it is not surprising that it will contain information about resonances. $Z(t)$ is obviously a strongly continuous family of contraction operators. Moreover, if $\varphi, \psi \in \mathscr{K}$ and $t, s \geq 0$, then $U(t)\varphi \in D_+^\perp$ and $U(-s)\psi \in D_-^\perp$ (since $U(t)$ leaves $D_\pm$ invariant for $\pm t \geq 0$). So

$$(U(-s)\varphi, P_\mathscr{K} U(t)\psi) = (U(-s)\varphi, U(t)\psi), \qquad t, s \geq 0$$

since $P_\mathscr{K} = P_- P_+$ where P_+ (respectively, P_-) is the projection onto the orthogonal *complement* of D_+ (respectively, D_-). Equivalently, $P_\mathscr{K} U(s) P_\mathscr{K} U(t) P_\mathscr{K} = P_\mathscr{K} U(s + t) P_\mathscr{K}$ or $Z(t)Z(s) = Z(t + s)$. Thus, $Z(t)$ is a strongly continuous group of contractions on $\mathscr{K}$, and therefore there is an m-accretive operator B on $\mathscr{K}$ with $\sigma(B) \subset \{z \mid \operatorname{Re} z > 0\}$ such that

$$Z(t) = e^{-Bt}$$

Since $U(t)$ has absolutely continuous spectrum,

$$(Z(t)\varphi, \psi) \to 0 \qquad \text{as} \quad t \to \infty \tag{223}$$

Moreover

$$Z(t) = P_+ U(t) P_-, \qquad t \geq 0 \tag{224}$$

For since $U(t)$ leaves D_+ invariant, $P_+ U(t) P_+ = P_+ U(t)$; and since $U(-t)$ leaves D_- invariant, $P_- U(t) P_- = U(t) P_-$; so

$$P_\mathscr{K} U(t) P_\mathscr{K} = P_- P_+ U(t) P_+ P_- = P_+ P_- U(t) P_- = P_+ U(t) P_-$$

The semigroup $Z(t)$ is important because the resolvent set of B is simply related to the invertibility of $s(z)$.

Theorem XI.90 Let D_+ and D_- be orthogonal outgoing and incoming subspaces for a unitary group $U(t)$ on a Hilbert space $\mathscr{H}$. Let $Z(t) = e^{-Bt}$ be defined by (222). Then, if $\operatorname{Re} z > 0$, $z \in \rho(B)$ if and only if $s(i\bar{z})$ is regular.

We shall sketch the proof that $s(i\bar{z}_0)^*$ has a zero eigenvalue if and only if B has z_0 as an eigenvalue. By definition,

$$\begin{aligned}\mathscr{K} &= \{\chi \mid \mathscr{R}_+ \chi \in L^2(-\infty, 0; N);\ \mathscr{R}_- \chi \in L^2(0, \infty; N)\} \\ &= \{\chi \mid \mathscr{R}_+ \chi \in L^2(-\infty, 0; N);\ \tilde{S}(\mathscr{R}_- \chi) = \mathscr{R}_+ \chi \in \tilde{S}L^2(0, \infty; N)\}\end{aligned}$$

Thus

$$\mathscr{R}_+[\mathscr{K}] \equiv \mathscr{K}_+ = \{f \mid f \in L^2(-\infty; 0; N),\ \tilde{S}^* f \in L^2(0, \infty; N)\}$$

Next, let $Z_+(t) = \mathscr{R}_+ Z(t) \mathscr{R}_+^{-1}$ and note that for $f \in \mathscr{K}_+$,

$$\begin{aligned}Z_+(t)f &= (\mathscr{R}_+ P_+ \mathscr{R}_+^{-1})(T_0(t)f) \\ &= \chi_{(-\infty, 0)} T_0(t) f\end{aligned}$$

That is, if $f \in \mathscr{K}_+$,

$$(Z_+(t)f)(s) = \begin{cases} f(s - t), & \text{if} \quad s \leq 0 \\ 0, & \text{if} \quad s > 0 \end{cases}$$

Now, $Bx = z_0 x$ if and only if $Z(t)x = e^{-z_0 t}x$. Moreover, $f(s-t) = e^{-z_0 t}f(s)$ $(s \le 0)$ if and only if $f(s) = e^{z_0 s}\chi_{(-\infty,0)}(s)n$ for some $n \in N$. Thus z_0 is an eigenvalue of B if and only if $e^{z_0 s}\chi_{(-\infty,0)}(s)n \equiv f_0$ is in $\mathscr{K}_+$ for some $n \in N$. Since f_0 is clearly in $L^2(-\infty, 0; N)$, $f_0 \in \mathscr{K}_+$ if and only if $\tilde{S}^* f_0$ is in $L^2(0, \infty; N)$. This is true if and only if $s(\bar{z})^* \hat{f}_0(z)$ is analytic in the lower half-plane. But $\hat{f}_0(z) = (2\pi)^{-1/2}(z_0 - iz)^{-1}n$ has a pole at $z = -iz_0$, so $s(\bar{z})^* \hat{f}_0(z)$ will be analytic in the lower half-plane if and only if $s(i\bar{z}_0)^* n = 0$. This completes the proof of one part of Theorem XI.90 and illustrates the reasons the theorem is valid.

Example 3 We consider a trivial example to illustrate Theorem XI.90. Let $U(t)$ be translation on $L^2(-\infty, \infty)$. Fix $r_0 > 0$, and let $D_+ = L^2(r_0, \infty)$, $D_- = L^2(-\infty, -r_0)$. Then D_+ is outgoing, D_- is incoming and, by a simple calculation, $\tilde{S} = U(-2r_0)$ and $s(k) = e^{2ikr_0}$. s is clearly entire. Notice that D_+ and D_- are orthogonal and that $\mathscr{K} = L^2(-r_0, r_0)$. It follows that $Z(t) = 0$ if $t > 2r_0$. In particular,

$$(B + \lambda)^{-1} = \int_0^\infty Z(t)e^{-\lambda t}\, dt$$

extends from $\operatorname{Re} \lambda > 0$ to an entire function. Thus $\sigma(B) = \varnothing$ which is as required by Theorem XI.90.

Theorem XI.90 reduces the analyticity question to studying B.

Theorem XI.91 Suppose that for some positive T and k, $Z(T)(k + B)^{-1}$ is compact. Then B has pure point spectrum and $s(z)$ is holomorphic on the real axis and has a meromorphic extension to the lower half-plane, having a pole at each z for which $iz \in \sigma(B)$.

The idea of the proof of this theorem is to use a spectral mapping theorem to show that B has pure point spectrum. By Theorem XI.90, $s(z)$ is invertible in the upper half-plane except when $i\bar{z}$ is an eigenvalue for B. Thus

$$s(z) = [s(\bar{z})^*]^{-1}$$

is analytic in the lower half-plane except for z for which iz is an eigenvalue of B. By the above expression, $s(z)$ can only have poles since $s(\bar{z})^*$ can only have zeros of finite order. Finally, by (223), B cannot have any eigenvalues with $\operatorname{Re} \mu = 0$. From this it follows that $(s(\bar{z})^*)^{-1}$ is analytic in an open set just below the real axis. Since $s(z)$ and $(s(\bar{z})^*)^{-1}$ have the same bounded boundary values as one approaches the real axis from above and below, they are analytic continuations of each other by the Schwartz reflection principle. Thus $s(z)$ is analytic in a neighborhood of the real axis and meromorphic in the lower half-plane.

For complete proofs of Theorems XI.90 and XI.91, see the reference in the Notes.

Example 4 The purpose of this example is to show how the hypotheses of Theorem XI.91 may be verified in practice. We shall deal with the case of scattering off an obstacle Ω with smooth boundary and Dirichlet boundary conditions discussed in Example 3 of Section 10. We use the notation introduced there. The operator A_1 for this problem is the Laplacian $H_{\Gamma;D}$ of Section XIII.15. We prove the absence of singular continuous spectrum in an appendix to this section. With this result, the analysis of Example 2 extends to this case. In their treatment, Lax and Phillips do not require a priori the absence of singular continuous spectrum. Instead, they prove (3) by a more difficult argument and then obtain the absence of singular continuous spectrum as a result of Theorem XI.82. The technique that we describe here can also be used to prove the hypotheses of Theorem XI.91 in the case of scattering in an inhomogeneous medium (Example 2), but the proofs are more difficult because the natural identification operator is not isometric (Problem 124).

D_+ and D_- are, as in Example 1, the incoming and outgoing subspaces for the free propagation $W_0(t)$. Let r_0 be chosen so that the ball $B(r_0)$ contains Ω in its interior and define

$$D_+^{r_0} = W_0(r_0)D_+, \qquad D_-^{r_0} = W_0(-r_0)D_-$$

Since the functions in $D_+^{r_0}$ and $D_-^{r_0}$ vanish in $B(r_0)$, $D_+^{r_0}$ and $D_-^{r_0}$ are subspaces of $\mathscr{H}_0$ that are isometrically imbedded in $\mathscr{H}_1$. One can show that $D_+^{r_0}$ and $D_-^{r_0}$ are outgoing and incoming subspaces for $W_1(t)$ on $\mathscr{H}_1$ and that the hypotheses of Theorem XI.86 hold. In particular, $D_\pm^{r_0}$ are orthogonal. Let $P_\pm^{r_0}$ be the projections onto $(D_\pm^{r_0})^\perp$ in $\mathscr{H}_1$ and define $Z(t) = P_+^{r_0} W_1(t) P_-^{r_0}$. Suppose that $\varphi \in \mathscr{H}_1$ and $\mu > 0$. Then, by (X.98),

$$\begin{aligned}
Z(2r_0)(\mu + B)^{-1}\varphi &= \int_0^\infty e^{-\mu t} Z(t + 2r_0)\varphi\, dt \\
&= P_+^{r_0} W_1(2r_0) \int_0^\infty e^{-\mu t} W_1(t) P_-^{r_0}\varphi\, dt \\
&= iP_+^{r_0} W_1(2r_0)(i\mu - A_1)^{-1} P_-^{r_0}\varphi \\
&= iP_+^{r_0} W_1(2r_0) P_-^{r_0}(i\mu - A_1)^{-1} P_-^{r_0}\varphi \qquad (225) \\
&= iP_+^{r_0}[W_1(2r_0) - W_0(2r_0)]P_-^{r_0} \\
&\quad \times (i\mu - A_1)^{-1} P_-^{r_0}\varphi \qquad (226) \\
&= iP_+^{r_0}[W_1(2r_0) - W_0(2r_0)] \\
&\quad \times (i\mu - A_1)^{-1} P_-^{r_0}\varphi \qquad (227)
\end{aligned}$$

Steps (225) and (227) follow from the fact that for $t \geq 0$, $P_-^{r_0} W_1(t) P_-^{r_0} = W_1(t) P_-^{r_0}$, from which it follows that

$$P_-^{r_0}(i\mu - A_1)^{-1} P_-^{r_0} = (i\mu - A_1)^{-1} P_-^{r_0}$$

Step (226) holds because $P_+^{r_0} W_0(2r_0) P_-^{r_0} = 0$. To see this notice that for any $f \in \mathscr{H}_1$, $P_-^{r_0} f$ is orthogonal to $D_-^{r_0}$ in $\mathscr{H}_0$ because $\mathscr{H}_1$ is isometrically imbedded in $\mathscr{H}_0$. Thus the free translation representative of $P_-^{r_0} f$ has support on $(-r_0, \infty)$. Therefore, the representative of $W_0(2r_0) P_-^{r_0} f$ has support on (r_0, ∞), which implies that $W_0(2r_0) P_-^{r_0} f$ is in $D_+^{r_0}$.

Now, for any $g \in \mathscr{H}_1$,

$$W_0(2r_0)g - W_1(2r_0)g = 0 \qquad \text{for} \quad |x| \geq 3r_0$$

since the propagation speed is one. Thus, using the fact that $\|\psi\|_0 = \|\psi\|_1$, we can estimate

$$\begin{aligned}
\|Z(2r_0)(\mu + B)^{-1}\varphi\|_1 &\leq \|[W_1(2r_0) - W_0(2r_0)](i\mu - A_1)^{-1} P_-^{r_0}\varphi\|_0 \\
&= \|[W_1(2r_0) - W_0(2r_0)](i\mu - A_1)^{-1} P_-^{r_0}\varphi\|_0^{(3r_0)} \\
&\leq \|W_1(2r_0)(i\mu - A_1)^{-1} P_-^{r_0}\varphi\|_1^{(3r_0)} \\
&\quad + \|W_0(2r_0)(i\mu - A_1)^{-1} P_-^{r_0}\varphi\|_0^{(3r_0)} \\
&\leq \|(i\mu - A_1)^{-1} P_-^{r_0}\varphi\|_1^{(5r_0)} + \|(i\mu - A_1)^{-1} P_-^{r_0}\varphi\|_0^{(5r_0)} \\
&= 2\|(i\mu - A_1)^{-1} P_-^{r_0}\varphi\|_1^{(5r_0)}
\end{aligned}$$

where $\|\cdot\|^{(R)}$ denotes the part of the norm inside the ball of radius R. In the next to last step we used part (a) of Lemma 1 in Example 2 and an analogous result for $W_1(t)$ (the proof is similar). The set of $\psi = (i\mu - A_1)^{-1}\varphi$ where $\|\varphi\| \leq 1$, satisfies

$$\|A_1\psi\|_1 + \|\psi\|_1 \leq \|A_1(i\mu - A_1)^{-1}\|_{\mathscr{L}(\mathscr{H}_1)} + \|(i\mu - A_1)^{-1}\|_{\mathscr{L}(\mathscr{H}_1)}$$

Therefore, using Corollary 2 to Theorem XIII.74, we see that the set of such ψ is compact in the $\|\cdot\|_1^{(5r_0)}$ norm. Thus, $Z(2r_0)(\mu + B)^{-1}$ is a compact operator, and so the hypotheses of Theorem XI.91 are satisfied.

The situation in this example has been studied in great detail and much more information is known. For example, $\mu \in \sigma(B)$ if and only if the reduced wave equation

$$\begin{aligned}
\Delta v - \mu^2 v &= 0 \\
v &= 0 \qquad \text{on } \partial D
\end{aligned} \tag{228}$$

has a solution v so that the data $\langle v, -\mu v\rangle$ is eventually outgoing, that is, satisfies $W_0(\rho)\langle v, -\mu v\rangle \in D_+$ for ρ large enough. The detailed relationship

between these eigenvalues and the geometry of the obstacle has been the object of much study. Finally, the scattering operator $\hat{S}$ has the form (recall that $N = L^2(S^2)$)

$$\begin{aligned}
(\hat{S}f)(\sigma, \omega) &= s(\sigma) f(\sigma, \omega) \\
&= f(\sigma, \omega) - \frac{i\sigma}{2\pi} \int_{|\theta| = 1} \overline{k(\theta, \omega; \sigma)}\, f(\sigma, \theta)\, d\theta
\end{aligned}$$

where $k(\theta, \omega; \sigma)$ is an analytic function of its variables which is related to the asymptotic behavior of the solutions of (228). This relationship is identical to the one between the quantum-mechanical T-matrix and the asymptotics of the solutions of the Lippmann–Schwinger equation.

It is clear from Examples 1, 2, and 4 that the Lax–Phillips method applies most naturally to classical wave equations where one has Huygens' principle, that is, in odd dimensions greater than one. Nevertheless, the theory can be applied in a variety of other situations as well (see the Notes for references).

Example 5 (application to the Schrödinger equation) As a last example we shall discuss how one can use the Lax–Phillips theory to study scattering for

$$i\frac{\partial u}{\partial t} = (-\Delta + V)u$$

The basic idea is to use the invariance principle for wave operators for the wave operators of the classical system

$$\begin{aligned}
u_{tt} - \Delta u + V(x)u &= 0 \\
u(x, 0) = f(x), \qquad u_t(x, 0) &= g(x)
\end{aligned} \tag{229}$$

We shall not obtain any results on the quantum-mechanical scattering operator that we have not already obtained in greater generality in Sections 4, 6, and 7, but it is interesting to get the results in a new way. We also emphasize that we shall need detailed spectral information about $-\Delta + V$ in order to apply the Lax–Phillips theory.

Let $V(x)$ be a potential with compact support in $\mathbb{R}^3$ and suppose that $V(x) \in L^2(\mathbb{R}^3)$ and $V(x) \geq 0$. First we want to solve (229). This is done analogously to the case of an inhomogeneous medium. Since $V \in L^2$, V is $-\Delta$-bounded (see Theorem X.15) so $-\Delta + V(x)$ is essentially self-adjoint. Further

$$((-\Delta + V)h, h) \geq (-\Delta h, h) \geq 0$$

so if $B_1 = \sqrt{-\Delta + V}$, we have $\|B_1 h\|_2 \geq \|B_0 h\|_2$. Moreover, $\mathscr{H}_1 \equiv [D(B_1)] \oplus L^2(\mathbb{R}^3) = \mathscr{H}_0$ since $-\Delta$ and $-\Delta + V$ have equal form domains. As before, if we define $W_1(t) = e^{-iA_1 t}$ where

$$A_1 = i\begin{pmatrix} 0 & I \\ -B_1^2 & 0 \end{pmatrix}$$

then the first component of $W_1(t)\langle f, g\rangle$ is a weak solution of (229) and a classical solution if f, g, and V are smooth enough.

The verification of hypotheses (i)–(iii) is analogous to Examples 2 and 4. Choose r_0 so that the ball $B(r_0)$ contains the support of $V(x)$ in its interior. Define $J: \mathscr{H}_0 \to \mathscr{H}_1$ to be the identity on those $\varphi \in \mathscr{H}_0$ with support outside $B(r_0)$ and any bounded injection on the orthogonal complement of this set. Finally, we take $D_+^{r_0}$ and $D_-^{r_0}$ to be $W_0(r_0)D_+$ and $W_0(-r_0)D_-$. As in the previous examples, properties (i) and (ii) for $U_1(t)$ and the orthogonality of $D_+^{r_0}$ and $D_-^{r_0}$ just follow from the corresponding properties of $W_0(t)$. Thus, if we can prove (iii), then we have verified the hypotheses of Theorem XI.86. To prove (iii) notice that the solutions of (229) propagate at speed one, so Lemmas 1 and 2 of Example 2 go through as before and the local compactness result of Lemma 3 is the same. Therefore, we need only show that $-\Delta + V$ has only absolutely continuous spectrum, and this is done by appealing to the same theorems that we appealed to in Example 2. Thus, by Theorem XI.82, we have the Lax–Phillips scattering operators S, $\tilde{S}$, and $\hat{S}$. By Theorem XI.86, $\Omega^{\pm}$ exist, are complete, and (215) holds.

An argument similar to that in Example 4 shows that $Z(2r_0)(\mu + B)^{-1}$ is compact for $\operatorname{Re}\mu > 0$ where $Z(t) = P_+ W_1(t) P_-$ and B is its generator. Thus $(\hat{S}f)(\sigma) = s(\sigma)f(\sigma)$ for all $f \in L^2(\mathbb{R}; S^2)$ where $s(\sigma)$ is meromorphic in the whole plane (with poles as singularities) and analytic on the real axis and in the upper half-plane.

Notice that for all data $\varphi \in C_0^\infty(\mathbb{R}^3) \times C_0^\infty(\mathbb{R}^3)$ and $|t|$ sufficiently large,

$$W_1(-t)JW_0(t)\varphi = W_1(-t)W_0(t)\varphi$$

and is independent of t. Just as in Examples 2 and 4, this follows because $W_0(t)$ satisfies Huygens' principle. Using Theorem XI.23, we conclude that the strong limits

$$\Omega^{\pm} = \operatorname*{s-lim}_{t \to \mp\infty} e^{+iA_1 t} e^{-iA_0 t}$$

exist and equal the wave operators already defined when applied to functions $\varphi \in E_{[0,\infty)}(A_0)$. But

$$A_0^2 = \begin{pmatrix} -\Delta & 0 \\ 0 & -\Delta \end{pmatrix}$$

and

$$A_1^2 = \begin{pmatrix} -\Delta + V & 0 \\ 0 & -\Delta + V \end{pmatrix}$$

Thus

$$\Omega^{\pm} = \begin{pmatrix} \Omega_S^{\pm}(-\Delta + V, -\Delta) & 0 \\ 0 & \Omega_S^{\pm}(-\Delta + V, -\Delta) \end{pmatrix}$$

Therefore, the Schrödinger wave operators exist and are complete.

Further development shows that the fibers of the Schrödinger S-operator are given by

$$e^{-i2r_0 E} s(\sqrt{E})$$

where $s(\cdot)$ are the $\mathscr{L}(L^2(S^2))$ fibers of the Lax–Phillips operator $\tilde{S}$. From the properties of $s(\cdot)$ discussed above it follows that $e^{i2r_0 E} s(\sqrt{E})$ is meromorphic on a two-sheeted Riemann surface, analytic on the "physical" sheet with poles on the "unphysical sheet."

Before concluding this example, it is worthwhile to make several remarks. First, notice that we needed quite a bit of sophisticated information about the interacting system, namely the character of $\sigma(-\Delta + V)$ in order to use the Lax–Phillips approach. Secondly, we have handled only the case $V \in L^2$, $V \geq 0$, and V has compact support. The restriction $V \in L^2$ is not serious. The second restriction can be avoided by a generalization of the ideas above. The reason we needed $V \geq 0$ was so that we could take the square root of $-\Delta + V$. But if $V \in L^2$ with compact support, then $-\Delta + V$ has at most finitely many negative eigenvalues (Theorem XIII.6) and on the complement of the space spanned by their eigenfunctions, $-\Delta + V$ will be nonnegative. One can then push through the technique of this example and one finds, as expected, that $e^{-i2r_0 E} s(\sqrt{E})$ has additional poles on the physical sheet at precisely the negative eigenvalues. The third restriction, that V have compact support, is much more serious since no potential in nature is believed to have compact support. And, it is crucial to all we have done in this section that the free and interacting systems are *identical* outside a bounded region.

Appendix to Section XI.11: The twisting trick

In this appendix we want to show that the Dirichlet Laplacian, $H_{D;\Gamma}$, exterior to a bounded region has empty singular continuous spectrum. We shall use a method (the twisting trick) which is applicable in a variety of other situations; see the reference in the Notes.

Theorem XI.91.5 Let Γ be a closed bounded set in $\mathbb{R}^n$ so that $\mathbb{R}^n\backslash\Gamma$ is connected. Let $H_{D;\Gamma}$ be the Dirichlet Laplacian defined in Section XIII.15. Fix $a > 0$. Let $X_a^{(\Gamma)}$ be the Hilbert space of functions $f \in L^2(\mathbb{R}^n\backslash\Gamma)$ with $e^{a|x|}f \in L^2$. Then, there is a set, $\mathscr{E}$, discrete in $\mathbb{R}\backslash\{0\}$, and a neighborhood N of $\mathbb{R}$ so that $(H_{D;\Gamma} - k^2)^{-1}$ can be extended as an analytic $\mathscr{L}(X_a^{(\Gamma)}, X_{-a}^{(\Gamma)})$-valued function from the region $\{k \mid \operatorname{Im} k > 0\}$ to $N\backslash\mathscr{E}$. In particular, $H_{D;\Gamma}$ has purely absolutely continuous spectrum.

Proof Since $\mathbb{R}^n\backslash\Gamma$ is connected, $H_{D;\Gamma}$ has no positive eigenvalues by the argument in Theorem XIII.56 (see especially the discussion preceding Theorem XIII.57). By Theorem XIII.20, the assertion about $\mathscr{L}(X_a^{(\Gamma)}, X_{-a}^{(\Gamma)})$ analyticity in $N\backslash\mathscr{E}$ shows that $\sigma_{\text{sing}}(H_{D;\Gamma}) = \varnothing$ since we can take X_a to be the dense set D and $[a, b]$ to be any closed interval disjoint from $\mathscr{E}$. Since $H_{D;\Gamma} \geq 0$ with empty kernel, $H_{D;\Gamma}$ clearly has no nonpositive eigenvalues. Thus, if we can prove the X_a assertion we will have a proof that the spectrum is purely absolutely continuous.

Define the operator H_α on $\mathscr{H} = L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n\backslash\Gamma)$ by

$$H_\alpha\langle\varphi, \psi\rangle = \langle(-\Delta + \alpha x^2)\varphi, H_{D;\Gamma}\psi\rangle$$

Suppose that $(H_\alpha - k^2)^{-1}$ has an $\mathscr{L}(X_a \oplus X_a^{(\Gamma)}, X_{-a} \oplus X_{-a}^{(\Gamma)})$ continuation onto $N_\alpha\backslash\mathscr{E}_\alpha$ where each $\mathscr{E}_\alpha$ may have some finite accumulation points but so that for any $\varepsilon > 0$ and $a > 0$, we can find an α so that $[\mathscr{E}_\alpha \cap (-a, a)]\backslash(-\varepsilon, \varepsilon)$ is a finite set. Then the result follows easily.

Define a "twisting operator" U on $\mathscr{H}$ as follows. Choose R so that $\Gamma \subset \{x \mid |x| < R\}$ and choose a C^∞, 2×2 unitary-matrix-valued function on $\mathbb{R}^n$, $u(x)$, so that

$$u(x) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{if} \quad |x| > 2R$$

$$u(x) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{if} \quad |x| < R$$

Define $(U\psi)(x) = u(x)\psi(x)$. Then U is unitary on $\mathscr{H}$ and on $X_{\pm a} \oplus X_{\pm a}^{(\Gamma)}$, so it suffices to prove the claimed continuation property for $UH_\alpha U^{-1}$. But $\tilde{H}_\alpha \equiv UH_\alpha U^{-1} = T_\alpha + V_\alpha$ where

$$T_\alpha\langle\varphi, \psi\rangle = \langle -\Delta\varphi, (H_{D;\Gamma} + \alpha x^2)\psi\rangle$$

$$V_\alpha = f_\alpha \cdot p + g_\alpha$$

where $p = i^{-1}\nabla$ and f_α and g_α are 2×2 matrices of C_0^∞ functions. Let $S_\alpha = \sigma(H_{D;\Gamma} + \alpha x^2)$ which is discrete (see Section XIII.14). By the analysis in the appendix to Section XI.6 (see especially Theorem XI.45), $(\tilde{H}_\alpha - k^2)^{-1}$ has an $\mathscr{L}(X_a, X_{-a})$ continuation to $N_\alpha\backslash\mathscr{E}_\alpha$ where the only possible limit points of N_α lie in $S_\alpha \cup \{0\}$, because $(T_\alpha - k^2)^{-1}$ has such a continuation on $\{k \mid \operatorname{Im} k > -a, \arg k \neq -\pi/2\}\backslash S_\alpha$. But $\inf S_\alpha \geq \inf(-\Delta + \alpha x^2)$ goes to infinity as $\alpha \to \infty$, so we can pick α so that $[\mathscr{E}_\alpha \cap (-a, a)]\backslash(-\varepsilon, \varepsilon)$ is finite. ∎

XI.12 The linear Boltzmann equation

In this section we describe a mathematical model for the scattering of a low-density beam of neutrons off a chunk of material such as uranium in free space. This model has only limited physical interest since it does not cover the nonscattering case where the number of neutrons grows exponentially in time, that is, the uranium blows up, nor the case where the neutron beam is constrained by shielding to stay in a bounded region filled with uranium and graphite rods, that is, a reactor. However, the model we describe is mathematically quite interesting since it provides a situation where the Hilbert space scattering theory must be extended in two ways: In the first place, the natural space of states is not a Hilbert space but a cone in a (non-Hilbert) vector space; in the second place, the equation of motion we describe defines a one-sided dynamics since the quantum aspects of the problem are modeled on a classical level by using statistical ideas. Moreover, the theory illustrates the natural use of semigroups on a Banach space.

The basic dynamical object is a positive function $n(x, v)$ on $\mathbb{R}^3 \times \mathbb{R}^3$ representing the density of neutrons at a point $\langle x, v\rangle$ in phase space. For a suitable integer N_0,

$$N_0 \int_{A \times B} n(x, v)\, d^3x\, d^3v$$

represents the number of neutrons in the set A with velocities in the set B. Of course, if $n(x, v)$ is a function, the number cannot be integral for all A and B; put differently, $n(x, v)$ should really be $N_0^{-1} \sum_{i=1}^{N_0} \delta(x - x_i)\, \delta(v - v_i)$. But if N_0 is large (it is typically at least 10^{20} for realistic experiments), it is a reasonable approximation to take $n(x, v)$ as an L^1 function. Thus, it is natural to take L^1_+, the cone of *positive* functions on $\mathbb{R}^3 \times \mathbb{R}^3$, as the set states of the system.

The dynamical equation postulated for $n(x, v)$ is

$$\frac{d}{dt} n(x, v, t) = -v \cdot \nabla_x n(x, v, t) + \int k(x, v', v) n(x, v', t)\, dv' - \sigma_a(x, v) n(x, v, t) \tag{230}$$

which is called the **linear Boltzmann equation**. To understand its meaning, let us solve the equation when k and σ_a are zero. Let

$$[W_0(t)n](x, v) = n(x - vt, v) \tag{231}$$

Theorem XI.92 For each $p \in [1, \infty]$ and in particular for $p = 1$, $W_0(t)$ is a strongly continuous group of isometries on $L^p(\mathbb{R}^6)$ taking positive functions into positive functions. Moreover, on each L^p, $p < \infty$, $C_0^\infty(\mathbb{R}^6)$ is a core for the infinitesimal generator of $W_0(t)$ and $W_0(t) = e^{-tT_0}$ where

$$T_0 f = v \cdot \nabla_x f \tag{232}$$

for $f \in C_0^\infty$.

Proof All the statements follow immediately from (231) except for the core statement and (232). These follow from Theorem X.49 if one notices that, by (231), C_0^∞ is left invariant by $W_0(t)$, that $W_0(t)f$ is C^∞ in t for $f \in C_0^\infty$, and that

$$-\frac{d}{dt} W_0(t)f\Big|_{t=0} = v \cdot \nabla_x f \quad \blacksquare$$

Thus, the first term on the right-hand side of the linear Boltzmann equation (230) describes the free classical motion of a group of neutrons with no scattering, no absorption, and no production. The second term has a very simple interpretation. A neutron at point $\langle x, v' \rangle$ in phase space may, due to scattering or to some production process such as fission, become or produce a neutron with a different velocity v. The total rate of production by or scattering from a neutron at $\langle x, v' \rangle$ is given by

$$\sigma_p(x, v') = \int k(x, v', v)\, dv \tag{233}$$

Similarly, the last term on the right-hand side of (230) represents the loss of neutrons from a point $\langle x, v \rangle$ in phase space due to scattering into other points $\langle x, v' \rangle$ in phase space or due to absorbtion (for example, by graphite rods).

Throughout our discussion we shall make the following assumptions on k, σ_a, and σ_p.

Definition We say that the pair $\langle k, \sigma_a \rangle$ is **regular** if and only if:

(i) k is a nonnegative measurable function on $\mathbb{R}^9$ and σ_a is a nonnegative measurable function on $\mathbb{R}^6$.

(ii) For each $\langle x, v' \rangle$, $k(x, v', \cdot)$ is in L^1 and σ_a and σ_p are uniformly bounded functions on $\mathbb{R}^6$.

(iii) There is a compact set D in $\mathbb{R}^3$ so that $k(x, v, v')$ and $\sigma_a(x, v)$ vanish if $x \notin D$.

Before studying solutions and scattering theory for (230), we would like to make several comments about the form of the equation and about our assumptions of "regularity." (230) has a "probabilistic" or "statistical" nature in that we are interpreting the latter two terms in terms of a certain fraction of the particles at $\langle x, v \rangle$ being produced, scattered, or absorbed. One can understand this statistical element as entering from one of two sources: In the first place, even classically the positions of the uranium atoms are changing due to thermal motions; secondly, since at its base the scattering is quantum mechanical, it is intrinsically given by probabilities. While one can easily understand the probabilistic nature of the equation (230), it has some surprising consequences. For example, despite the fact that we are thinking of the equation as describing the motion of an aggregation of particles, each obeying a particle dynamics that is given by time reversible laws (Newton's equation), the equation (230), *as an equation on* L^1_+, is only solvable for positive times, as we shall see below.

The reason that the term "linear" is added to the name is that the original equations proposed by Boltzmann (to describe gases, not neutrons) contained a quadratic term in n due to the scattering of the basic particles off one another. In the "small" n limit this term is unimportant. Physically, "small" n means that the density of neutrons is low compared to the density of scattering objects and low enough so that it is unlikely that two neutrons get close enough to interact significantly. These assumptions are not unreasonable.

The assumption that σ_a and σ_p have bounded supports in the x variable is not really necessary for the mathematical theory although it is natural from a physical point of view. See the Notes for a reference that describes the scattering theory if σ_a and σ_p are only assumed to fall off sufficiently rapidly. We remark that σ does not stand for a cross section but for a rate.

There are three situations that have obvious physical interpretations. The first is where $\sigma_a(x, v) = \sigma_p(x, v)$ for all $x, v \in \mathbb{R}^6$. Here the number of neutrons that leave $\langle x, v \rangle$ is precisely equal to the number of neutrons that enter other regions of phase space due to the presence of neutrons at $\langle x, v \rangle$. For obvious reasons, this is called the **pure scattering case**. Similarly $\sigma_a \leq \sigma_p$ is called the **production case** and $\sigma_a \geq \sigma_p$ the **absorption case**.

Finally, we remark on the apparent lack of conservation of energy in (230). For we do not require k to be supported in the region where $|v| = |v'|$; in fact, since k is a function rather than a distribution or measure, k cannot be supported in that region without being zero almost everywhere.

One can develop the theory by replacing

$$\int k(x, v', v)n(x, v', t)\,dv' \qquad \text{by} \qquad \int k(x, |v|\Omega', v)n(x, |v|\Omega', t)\,d\Omega'$$

and this is appropriate in some ways in the pure scattering case. But there is a physical reason why a spread of final velocities is appropriate. For the uranium nuclei are not fixed, so the final velocity is dependent on the initial velocity of the uranium nuclei, even in elastic collisions. Since we "average" over positions of uranium nuclei in the statistical sense mentioned above, it is not unreasonable to "average" over velocities too.

Solving (230) is an exercise in the theory of semigroups on Banach spaces:

Theorem XI.93 Let $\langle k, \sigma_a \rangle$ be a regular pair. Then there exists a one-parameter strongly continuous semigroup $W(t)$, $t \geq 0$, on $L^1(\mathbb{R}^6)$ taking $L^1_+(\mathbb{R}^6)$ into itself, so that $W(t) = e^{-tT}$, with $C_0^\infty(\mathbb{R}^6)$ a core for T, and

$$Tf(x, v) = T_0 f(x, v) - \int k(x, v', v)f(x, v')\,dv' + \sigma_a(x, v)f(x, v)$$

Moreover:

(a) $D(T) = D(T_0)$.
(b) $\|W(t)\| \leq e^{Ct}$ with $C = \|\sigma_p\|_\infty$.
(c) In the pure scattering (respectively, absorption) case $\|W(t)n\|_1 = \|n\|_1$ (respectively, $\|W(t)n\|_1 \leq \|n\|_1$) for all $n \in L^1_+$.
(d) For any $n \in L^1_+$ and all $\langle x, v \rangle$ and $t > 0$,

$$[W(t)n](x, v) \geq n(x - tv, v) \exp\left(-\int_0^t \sigma_a(x - sv, v)\,ds\right) \tag{234}$$

Proof Define operators A_1, A_2 on $L^1(\mathbb{R}^6)$ by

$$(A_1 n)(x, v) = -\int k(x, v', v)n(x, v')\,dv'$$

$$(A_2 n)(x, v) = \sigma_a(x, v)n(x, v)$$

Then A_1 and A_2 are bounded with norms $\|\sigma_p\|_\infty$ and $\|\sigma_a\|_\infty$, respectively. Moreover, if $\tilde{T} = T_0 + A_2$, then $\tilde{W}(t) = e^{-t\tilde{T}}$ is given by the explicit formula

$$(\tilde{W}(t)n)(x, v) = n(x - tv, v) \exp\left(-\int_0^t \sigma_a(x - sv, v)\,ds\right) \tag{235}$$

Since $T = T_0 + A_1 + A_2$, it follows from Theorem X.50 that T generates an exponentially bounded semigroup, that any core for T_0 is one for T, and that $D(T) = D(T_0)$. Since $\|e^{-tA_1}\| \leq e^{t\|A_1\|}$ and $\|\tilde{W}(t)\| \leq 1$, it follows from the Trotter product formula (Theorem X.51) that

$$\|W(t)\| \leq \|e^{-tA_1}\| \leq \exp(t\|\sigma_p\|_\infty)$$

proving (b).

As in Section X.9 (step 4 in the proof of Theorem X.58), one verifies Duhamel's formulas:

$$W(t) = W_0(t) - \int_0^t W_0(t - s)(A_1 + A_2)W(s)\,ds \tag{236}$$

and

$$W(t) = \tilde{W}(t) - \int_0^t W(t - s)A_1 \tilde{W}(s)\,ds \tag{237}$$

Now $e^{-A_1 t}$ is positivity preserving since $-A_1$ is and one can expand the exponential. Thus, by the Trotter product formula, and the fact $\tilde{W}$ is obviously positivity preserving, we conclude that $W(t)$ takes L^1_+ into itself. Moreover, by (237) $W(t)n \geq \tilde{W}(t)n$ pointwise, which proves (234).

All that remains is part (c). Notice that

$$\int [W_0(t)n](x, v)\,dx\,dv = \int n(x, v)\,dx\,dv$$

$$\int (A_1 n)(x, v)\,dx\,dv = -\int \sigma_p(x, v')n(x, v')\,dx\,dv'$$

so, by (236) and properties of $W_0(t)$,

$$\int (W(t)n)(x, v)\,dx\,dv$$

$$= \int n(x, v)\,dx\,dv + \int_0^t ds \int [\sigma_p(x, v) - \sigma_a(x, v)](W(s)n)(x, v)\,dx\,dv \tag{238}$$

from which (c) follows immediately. ∎

We are now in a position to explain the sense in which the dynamical operator $W(t)$ is not invertible. As a map from L^1 to L^1 it is invertible since $-T_0 - A_1 - A_2$ generates a semigroup, but this inverse does not in general take L^1_+, the basic set of states, into itself; for an example of this phenomenon see the reference in the Notes. Given a one-sided dynamics $W(t)$

($t \geq 0$) and a two-sided comparison dynamics $W_0(t)$ ($-\infty < t < \infty$), it is fairly obvious that the natural scattering theory objects are

$$\Omega^+ = \text{s-lim}_{t \to -\infty} W(-t)W_0(t) \tag{239}$$

$$\tilde{\Omega}^- = \text{s-lim}_{t \to +\infty} W_0(-t)W(t) \tag{240}$$

$\Omega^+ n_0$ is the value at $t = 0$ of the solution of the interacting problem, which looks like $W_0(t)n_0$ in the distant past. And $\tilde{\Omega}^- n_1$ is the value at $t = 0$ for the free propagation, which looks more and more like $W(t)n_1$ as $t \to +\infty$. Thus, if Ω^+ and $\tilde{\Omega}^-$ exist, the scattering operator is given by

$$S = \tilde{\Omega}^- \Omega^+$$

Notice that (239) and (240) involve $W(t)$ only for t positive. On the basis of the examples we have previously discussed, we expect the existence of the limit (239) to be easier than that of (240).

Further, there are cases where one does not expect either of them to exist. For, if there is too much neutron production, the number of neutrons may grow indefinitely with time, in which case physically the uranium blows up and mathematically we are in a nonscattering situation. We therefore single out a class of interactions.

Definition We say that a regular pair $\langle k, \sigma_a \rangle$ is **subcritical** if and only if $\sup_{t \geq 0} \|W(t)\| < \infty$.

By (238), $\langle k, \sigma_a \rangle$ is subcritical in the pure scattering and absorbtive cases. We shall see below (Theorem XI.95) that it is also subcritical in the production case if the chunk of matter is sufficiently small.

The following simple geometric lemma is crucial both in controlling the limit (239) and in proving subcriticality in the small region production case. Intuitively, it says that the number of neutrons in a bounded region goes down quite fast as long as there are not too many with very small velocities to begin with.

Lemma For any Borel set $D \subset \mathbb{R}^3$, let $\|n\|_D = \int_{x \in D} \int_{\mathbb{R}^3} n(x, v)\, dx\, dv$. Then for $n \in L^1_+(\mathbb{R}^6)$

$$\int_{-\infty}^{\infty} \|W_0(t)n\|_D\, dt \leq (\text{diam } D)\|v^{-1}n\|_{L^1(\mathbb{R}^6)}$$

where diam $D = \sup_{x, y \in D} |x - y|$.

Proof It suffices to prove that for each fixed $v \neq 0$,

$$\int_{-\infty}^{\infty} \int_{x \in D} |W_0(t)n(x, v)|\, dx\, dt \leq [\text{diam } D] \int |v|^{-1} |n(x, v)|\, dx \tag{241}$$

Let χ be characteristic function of D. Then the left-hand side of (241) is $\int_{-\infty}^{\infty} (\int \chi(x) |n(x - vt, v)|\, dx)\, dt$. Let y be the component of x parallel to v and $x_\perp$ the two coordinates orthogonal. Then the last integral can be written

$$\int_{-\infty}^{\infty} dt \int dx_\perp \int dy\, \chi(y, x_\perp) |n(y - |v|t, x_\perp, v)|$$

$$= |v|^{-1} \int dz \int dx_\perp \int dy\, \chi(y, x_\perp) |n(z, x_\perp, v)|$$

$$\leq |v|^{-1} (\text{diam } D) \iint dx_\perp\, dz\, |n(z, x_\perp, v)|$$

proving (241). In the above, we changed variables from t to $z = y - |v|t$ in the first step and used the obvious geometric fact $|\int \chi(y, x_\perp)\, dy| \leq \text{diam } D$ in the second. ∎

Theorem XI.94 If $\langle k, \sigma_a \rangle$ is a regular pair defining a subcritical system, then Ω^+ exists and is a positivity preserving operator. Ω^+ is a contraction (respectively, isometry) in the absorbtion (respectively, pure scattering) case.

Proof Since $\langle k, \sigma_a \rangle$ is subcritical, the family $\{W(-t)W_0(t)\}$ is uniformly bounded. Thus, it suffices to prove that the limit (239) exists for a dense set $\mathscr{D}$ in L^1. The other properties of Ω^+ follow from those of $W(-t)$ and $W_0(t)$. Take

$$\mathscr{D} = \left\{ n \in C_0^\infty(\mathbb{R}^6) \,\middle|\, |v|^{-1} n \in L^1 \right\}$$

Let $A = A_1 + A_2$ as in Theorem XI.93 and let D be a bounded set containing supp σ_a and supp σ_p. Then for $n \in \mathscr{D}$,

$$\int_{-\infty}^{0} \|AW_0(t)n\|\, dt \leq \|A\| \int_{-\infty}^{0} \|W_0(t)n\|_D\, dt$$

$$\leq \|A\| (\text{diam } D) \|v^{-1}n\|_1 < \infty$$

by the lemma. By Cook's method, the limit (239) exists. ∎

We need a further condition on $\langle k, \sigma_a \rangle$ to make the interaction subcritical if the volume of matter is small. We say that $\langle k, \sigma_a \rangle$ has **finite mean free path** if

$$M(\sigma_p) \equiv \|v^{-1}\sigma_p\|_\infty < \infty$$

The reason for the name is that $(v^{-1}\sigma_p)^{-1}$ represents a distance between successive collisions or particle productions.

Theorem XI.95 A regular pair $\langle k, \sigma_a \rangle$ with finite mean free path that obeys (diam D)$M(\sigma_p) < 1$ is subcritical and, in particular, Ω^+ exists.

Proof Using (237) and the fact that $\tilde{W}(t)$ is a contraction, we easily obtain

$$\sup_{0 \le t \le T} \|W(t)\| \le 1 + \alpha \sup_{0 \le t \le T} \|W(t)\|$$

where

$$\alpha \equiv \int_0^\infty \|A_1 \tilde{W}(s)\| \, ds$$

Thus, if $\alpha < 1$,

$$\sup_{0 \le t < \infty} \|W(t)\| \le (1 - \alpha)^{-1}$$

and the system is subcritical. Therefore, we need only prove that

$$\alpha \le (\text{diam } D) M(\sigma_p) \tag{242}$$

Since $\|A_1 v^{-1}\|_{op} = M(\sigma_p)$, (242) follows if we prove that

$$\int_0^\infty \|v\tilde{W}(s)n\|_D \, ds \le (\text{diam } D)\|n\|_1$$

But v commutes with $\tilde{W}(s)$ and $\|\tilde{W}(s)n\|_D \le \|W_0(s)n\|_D$, so, by the lemma,

$$\int_0^\infty \|v\tilde{W}(s)n\|_D \, ds \le (\text{diam } D)\|vv^{-1}n\|_1$$

This proves (242) and thus the theorem. ∎

Basically, the condition $\alpha < 1$ in the proof implies that the iteration of (237) converges uniformly in t. The physical reason for this is that (diam D)$M(\sigma_p) < 1$ says that, to first order, a particle passing through D undergoes less than one collision and so the geometric series obtained by iterating and using $\alpha < 1$ converges. We note that Theorem XI.95 provides us with a large variety of semigroups bounded in time which are not contraction semigroups. With one more condition we can now prove the existence of the limit (240).

Theorem XI.96 Suppose that the system defined by the regular pair $\langle k, \sigma_a \rangle$ has finite mean free path, is subcritical, and that

$$M(\sigma_a) \equiv \|v^{-1}\sigma_a\|_\infty < \infty$$

Then $\tilde{\Omega}^-$ exists. The scattering operator $S = \tilde{\Omega}^- \Omega^+$ is a bounded one-to-one map of $L^1_+(\mathbb{R}^6)$ into itself.

Proof Let $\sigma_1 = \sigma_p$ and $\sigma_2 = \sigma_a$. We first claim that for all $\langle x, v \rangle \in \mathbb{R}^6$,

$$\int_0^\infty \sigma_i(x - sv, v) \, ds \le [\text{diam } D] M(\sigma_i) \tag{243}$$

(243) is proven just as in the proof of the lemma. By (d) of Theorem XI.93 and (243),

$$(W(t)n)(x, v) \ge \exp(-[\text{diam } D]M(\sigma_2))n(x - vt, v)$$

for n positive. Letting $C = \exp([\text{diam } D]M(\sigma_2))$, we have

$$n(x, v) \le C(W(t)n)(x + vt, v) \tag{244}$$

Thus, replacing n by $W(s)n$ and t by $t - s$,

$$(W(s)n)(x, v) \le C(W(t)n)(x + v(t - s), v)$$

Therefore, for n positive,

$$\begin{aligned}
\int_0^t \|A_i W(s)n\|_1 \, ds &= \int_0^t ds \int \sigma_i(x, v)(W(s)n)(x, v) \, dx \, dv \\
&\le C \int_0^t ds \int \sigma_i(x, v)(W(t)n)(x + v(t - s), v) \, dx \, dv \\
&= C\left(\int_0^t \sigma_i(y - vr, v) \, dr\right) \int (W(t)n)(y, v) \, dy \, dv \\
&\le C(\text{diam } D) M(\sigma_i) \|W(t)n\|_1
\end{aligned}$$

In the next to last step we changed variables in two places and in the last step used (243). It follows that

$$\int_0^\infty \|A_i W(s)n\|_1 \, ds \le C[\text{diam } D] M(\sigma_i) \sup_{t \ge 0} \|W(t)n\|_1$$

As a result, subcriticality implies that

$$\int_0^\infty \|A_i W(s)n\|_1 \, ds < \infty$$

which by Cook's method implies the existence of the limit (240). Ω^+ exists by Theorem XI.94; and since $\{W(t)\}$ is uniformly bounded and each $W(t)$ is positivity-preserving, Ω^+, $\tilde{\Omega}^-$ are bounded positivity-preserving operators on $L^1_+(\mathbb{R}^6)$. Therefore, the same is true of $S = \tilde{\Omega}^- \Omega^+$. By (244)

$$\|W(t)n\|_1 \geq C^{-1}\|n\|_1$$

for n positive. From this and the fact that $W_0(t)$ is an isometry it easily follows that S is one-to-one. ∎

XI.13 Nonlinear wave equations

... formerly unsolvable equations are dealt with by threats of reprisals. *Woody Allen*

In this section we give an introduction to the scattering theory of nonlinear classical wave equations. There are many unsolved problems in this area, and the scattering theories that do exist are typically valid only for special nonlinear terms. The general ideas follow the outline given in Section 1, although the techniques for proving estimates are more difficult than in the linear case. Let us begin by looking at the equation

$$u_{tt} - \Delta u + m^2 u = F(u) \tag{245}$$

In Section X.13 we developed the existence theory for (245) for the case $F(u) = \pm\lambda|u|^{p-1}u$, where $p = 3$. The same method works for $p < 5$. To develop a scattering theory for (245) one might try to show that for large positive and negative times, its solutions look more and more like solutions of the corresponding free equation:

$$u_{tt} - \Delta u + m^2 u = 0 \tag{246}$$

The solutions of this free equation with nice initial data decay in the sup norm like $t^{-n/2}$ in n space dimensions (see Theorem XI.17). If the same decay holds for solutions of (245), a scattering theory should exist since a term like $-\lambda|u|^{p-1}u$ will decay faster than the linear terms if $p > 1$. However, even for the linear Schrödinger equation, one does not expect all solutions of the interacting equation to decay since there may be bound states. There should also be bound states for (245), at least for suitable F.

Suppose that F has the form $F(y) = yH(|y|)$ where $H(|y|) \to 0$ as $|y| \to 0$. Then (245) has a solution of the form

$$u_0(x, t) = e^{i\omega t}\varphi(x) \tag{247}$$

if and only if

$$-\Delta\varphi(x) + V(x)\varphi(x) = -(m^2 - \omega^2)\varphi(x) \tag{248a}$$

$$V(x) = -H(|\varphi(x)|) \tag{248b}$$

Except for very pathological potentials, the Schrödinger equation will not have positive eigenvalues (see Section XIII.13). Thus, we restrict our attention to the case $|\omega| < m$. If $V(x)$ is positive, for example if $F(u) = -\lambda u|u|^2$, then of course (248a) will have no such solutions since $-\Delta + V \geq 0$. If $V(x)$ is not always positive, then it is not surprising that solutions exist. In fact, the reference given in the Notes constructs large classes of F's with solutions of (248). An explicit example where such solutions exist is

$$F(u) = -u(|u|^2 - \lambda|u|)$$

for suitably large λ.

If solutions of the form (247) exist, then there should be solutions of (245) which look asymptotically (as $t \to -\infty$) like $u_0(x, t)$ plus a solution of (246). Since the nonlinearity couples the bound state to the asymptotically free piece, there is no reason to expect that the bound state will be present as $t \to +\infty$. Thus, if there are bound states, the scattering theory for (245) is intrinsically a multichannel problem. In fact, there should be an infinite number of channels. For, by the Lorentz invariance of (245), the existence of a u_0 implies the existence of a solution of (245) of the form

$$\exp(i(t - v^{-1}x)\omega(v))\psi(x - vt)$$

Thus it should be possible to construct solutions of (245) that consist of n bumps moving relative to one another. In addition to this there are examples with infinitely many bound states for fixed ω. And, one expects bound states for every sufficiently small ω.

Thus, not only is the problem nonlinear, but the full complexity of multichannel scattering is present. The two general cases where asymptotic completeness can be proven are precise analogues of the two cases where asymptotic completeness has been known for multichannel Schrödinger systems for many years. The small data case which we present first is the analogue of weak coupling (Theorem XIII.27). The result discussed at the end of the section is the analogue of the repulsive potential case (Theorem XIII.32). In the middle part of the section we present a general construction of the channel wave operators for the channel where u is asymptotically free.

It is also worth mentioning at the outset two technical difficulties that arise here but not in linear quantum-mechanical scattering. First, since the wave and scattering operators are nonlinear, in order to prove existence it is not sufficient to prove that they exist on a dense set and then extend by the B.L.T. theorem. Secondly, it is natural to take as scattering states the set of initial data Σ_{scat} for which the solutions of (246) decay appropriately at $\pm\infty$. Unfortunately, only sufficient conditions are known for such decay, so the norm on Σ_{scat} typically involves explicitly the large time behavior of the solution of the corresponding linear equation. This causes some technical complications.

In Section X.13 we showed that (245) can be reformulated as

$$\varphi'(t) = -iA\varphi(t) + J(\varphi(t)) \tag{249a}$$

where $J(\langle u, v\rangle) = \langle 0, F(u)\rangle$,

$$A = i\begin{pmatrix} 0 & I \\ \Delta - m^2 & 0 \end{pmatrix}$$

and $\varphi(t) = \langle u(\cdot, t), v(\cdot, t)\rangle$ is viewed as a function from $\mathbb{R}$ to $D((-\Delta + m^2)^{\frac{1}{2}}) \oplus L^2(\mathbb{R}^3)$. This led us to study the existence theory of (249a) as an abstract problem where $\varphi(t)$ takes values in a Hilbert space $\mathscr{H}$, A is self-adjoint on $\mathscr{H}$, and J is a nonlinear mapping of $\mathscr{H}$ into itself. Under the condition that J be uniformly Lipschitz on balls in $\mathscr{H}$ we proved that the corresponding integral equation

$$\varphi(t) = e^{-itA}\varphi_0 + \int_0^t e^{-iA(t-s)}J(\varphi(s))\,ds \tag{249b}$$

has a unique continuous $\mathscr{H}$-valued solution φ for small t. If J satisfies additional estimates and the initial data φ_0 are in $D(A)$, then we showed that φ is strongly differentiable and (249a) holds. In this section we shall always work with (249b); the reader should consult Section X.13 for the sufficient conditions that φ satisfy (249a).

We begin by presenting an abstract scattering theory for small data. Let A be a self-adjoint operator on $\mathscr{H}$. Let $\|\cdot\|_a$ and $\|\cdot\|_b$ be two auxiliary "norms" on $\mathscr{H}$: $\|\cdot\|_a$ satisfies all the properties of a norm except that $\|\varphi\|_a = 0$ need not imply that $\varphi = 0$; $\|\cdot\|_b$ satisfies all the properties of a norm except that it may take the value $+\infty$. We assume that A, J, and $\|\cdot\|_a$, $\|\cdot\|_b$ satisfy the following hypotheses:

(i) There is a $c > 0$ so that

$$\|\varphi\|_a \le c\|\varphi\| \qquad \text{for all} \quad \varphi \in \mathscr{H} \tag{250}$$

(ii) There are constants $c_1 > 0$, $d > 0$, so that for $\varphi \in \mathscr{H}$,

$$\|e^{-iAt}\varphi\|_a \le c_1 t^{-d}\|\varphi\|_b \qquad \text{if} \quad |t| \ge 1 \tag{251}$$

(iii) There exist $\beta > 0$, $\delta > 0$, and $q \ge 1$ with $dq > 1$, so that

$$\|J(\varphi_1) - J(\varphi_2)\| \le \beta(\|\varphi_1\|_a + \|\varphi_1\|_a)^q\|\varphi_1 - \varphi_2\| \tag{252}$$

$$\|J(\varphi_1) - J(\varphi_2)\|_b \le \beta\{(\|\varphi_1\|_a + \|\varphi_2\|_a)^{q-1}\|\varphi_1 - \varphi_2\|_a + (\|\varphi_1\|_a + \|\varphi_2\|_a)^q\|\varphi_1 - \varphi_2\|\} \tag{253}$$

for all $\varphi_1, \varphi_2 \in \mathscr{H}$ satisfying $\|\varphi_i\| \le \delta$. In the case $q = 1$ we assume that β can be chosen arbitrarily small if δ is chosen small. Moreover, we assume that $J(0) = 0$.

We can now define the scattering states and the scattering norm. First, for an $\mathscr{H}$-valued function $\psi(t)$ on $\mathbb{R}$ we define

$$|||\psi(\cdot)|||_{[N_1, N_2]} \equiv \sup_{N_1 \le t \le N_2} \|\psi(t)\| + \sup_{N_1 \le t \le N_2} (1 + |t|)^d\|\psi(t)\|_a$$

In the case where $N_1 = -\infty$, $N_2 = +\infty$ we shall denote the norm simply by $|||\cdot|||$. Now we define

$$\Sigma_{\text{scat}} \equiv \left\{\varphi \in \mathscr{H} \;\middle|\; |||e^{-itA}\varphi||| < \infty\right\}$$

and

$$\|\varphi\|_{\text{scat}} \equiv |||e^{-itA}\varphi|||$$

That is, the scattering states are just those vectors in $\mathscr{H}$ that decay nicely in the $\|\cdot\|_a$ norm under the free propagation. Notice that if $\|\varphi\|_b < \infty$, then

$$\|e^{-itA}\varphi\|_a \le c_2(1 + |t|)^{-d}(\|\varphi\| + \|\varphi\|_b) \qquad \text{for all } t \tag{254}$$

so $\varphi \in \Sigma_{\text{scat}}$ and

$$\|\varphi\|_{\text{scat}} \le (1 + c_2)\|\varphi\| + c_2\|\varphi\|_b$$

Theorem XI.97 (global existence for small data) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J be a nonlinear mapping of $\mathscr{H}$ into itself. Suppose that there exist $\|\cdot\|_a$, $\|\cdot\|_b$ so that hypotheses (i)–(iii) hold. Then there is an $\eta_0 > 0$ so that for all $\varphi_- \in \Sigma_{\text{scat}}$ with $\|\varphi_-\|_{\text{scat}} \le \eta_0$, the equation

$$\varphi(t) = e^{-itA}\varphi_- + \int_{-\infty}^t e^{-iA(t-s)}J(\varphi(s))\,ds \tag{255}$$

has a unique global continuous $\mathscr{H}$-valued solution φ with $|||\varphi(\cdot)||| \le 2\eta_0$. Moreover:

(a) For each t, $\varphi(t) \in \Sigma_{\text{scat}}$.
(b) $\|\varphi(t) - e^{-itA}\varphi_-\| \to 0$ as $t \to -\infty$.

Proof The basic idea is to use the contraction mapping method which we employed in Section X.13 except with initial conditions at $t = -\infty$. Thus, this theorem is similar to our discussion in Section 2. Let X_{η,φ_-} denote the set of continuous $\mathscr{H}$-valued functions $\psi(t)$ so that $|||\psi(t) - e^{-itA}\varphi_-||| \le \eta$. Assume that $\|\varphi_-\|_{\text{scat}} \le \eta \le \frac{1}{2}\delta$ where δ is chosen so that hypothesis (iii) holds. For $\psi(\cdot) \in X_{\eta,\varphi_-}$, define

$$(\mathscr{J}\psi)(t) = \int_{-\infty}^{t} e^{-iA(t-s)}J(\psi(s))\,ds$$

As in the proof of Theorem X.72, it is easy to check that $e^{-iA(t-s)}J(\psi(s))$ is a continuous function of s for each t. Further, since $\|\psi(s)\| \le |||\psi(\cdot)||| \le |||e^{-itA}\varphi_-||| + \eta \le 2\eta$, we have

$$\begin{aligned}\|J(\psi(s))\| &\le \beta\|\psi(s)\|_a^q\|\psi(s)\| \\ &\le \beta|||\psi(\cdot)|||^{q+1}(1 + |s|)^{-dq} \\ &\le \beta(2\eta)^{q+1}(1 + |s|)^{-dq}\end{aligned}$$

by (252), so

$$\begin{aligned}\|(\mathscr{J}\psi)(t)\| &\le \int_{-\infty}^{t} \|e^{-iA(t-s)}J(\psi(s))\|\,ds \\ &\le \beta(2\eta)^{q+1}\int_{-\infty}^{t}(1 + |s|)^{-dq}\,ds < \infty \qquad (256)\end{aligned}$$

since $dq > 1$. Also

$$\begin{aligned}\|(\mathscr{J}\psi)(t)\|_a &\le \int_{-\infty}^{t} \|e^{-iA(t-s)}J(\psi(s))\|_a\,ds \\ &\le c_2\int_{-\infty}^{t}(1 + |t-s|)^{-d}(\|J(\psi(s))\|_b + \|J(\psi(s))\|)\,ds \quad \text{(by (254))} \\ &\le c_2\beta\int_{-\infty}^{t}(1 + |t-s|)^{-d}\{\|\psi(s)\|_a^q(1 + 2\|\psi(s)\|)\}\,ds \\ &\qquad \text{(by (252) and (253))} \\ &\le c_2\beta(2\eta)^q(1 + 4\eta)\int_{-\infty}^{t}(1 + |t-s|)^{-d}(1 + |s|)^{-dq}\,ds \qquad (257) \\ &\le c_2\beta(2\eta)^q(1 + 4\eta)c_3(1 + |t|)^{-d}\end{aligned}$$

The last step follows from the lemma proved after the completion of this proof. Therefore $|||(\mathscr{J}\psi)(t)||| < \infty$. We now define

$$(\mathscr{M}\psi)(t) = e^{-iAt}\varphi_- + (\mathscr{J}\psi)(t)$$

and choose η_0 (and δ in the case $q = 1$) small enough so that

$$\begin{aligned}\beta(2\eta_0)^{q+1}\int_{-\infty}^{\infty}(1 + |s|)^{-dq}\,ds &\le \tfrac{1}{2}\eta_0 \\ c_2\beta(2\eta_0)^q(1 + 4\eta_0)c_3 &\le \tfrac{1}{2}\eta_0 \qquad (258)\end{aligned}$$

It is easy to check that $(\mathscr{M}\psi)(t)$ is continuous. Thus, for $\eta \le \eta_0$, $\mathscr{M}$ maps X_{η,φ_-} into itself. Further, it is easy to check using (253) that by choosing η_0 still smaller (and δ in the case $q = 1$) we can guarantee that $\mathscr{M}$ is a contraction. Thus, since X_{η,φ_-} is a complete metric space, $\mathscr{M}$ has a unique fixed point $\varphi(\cdot)$ in X_{η,φ_-}. By the definition of $\mathscr{M}$, $\varphi(\cdot)$ is a global solution of (255). Notice also that $|||\varphi(\cdot)||| \le 2\eta_0$.

To prove uniqueness, let φ_1 be another solution of (255) with $|||\varphi_1(\cdot)||| < \infty$. Then

$$\begin{aligned}\|\varphi(t) - \varphi_1(t)\| &\le \int_{-\infty}^{t}\|J(\varphi(s)) - J(\varphi_1(s))\|\,ds \\ &\le \int_{-\infty}^{t}\beta(\|\varphi(s)\|_a + \|\varphi_1(s)\|_a)^q\|\varphi(s) - \varphi_1(s)\|\,ds \\ &\le \beta(|||\varphi(\cdot)||| + |||\varphi_1(\cdot)|||)^q\Big(\sup_{-\infty<s\le t}\|\varphi(s) - \varphi_1(s)\|\Big) \\ &\quad \times \int_{-\infty}^{t}(1 + |s|)^{-dq}\,ds\end{aligned}$$

so

$$\begin{aligned}&\sup_{-\infty<s\le t}\|\varphi(s) - \varphi_1(s)\| \\ &\quad \le \Big\{\beta(|||\varphi(\cdot)||| + |||\varphi_1(\cdot)|||)^q\int_{-\infty}^{t}(1 + |s|)^{-dq}\,ds\Big\}\sup_{-\infty<s\le t}\|\varphi(s) - \varphi_1(s)\|\end{aligned}$$

But this gives a contradiction for t sufficiently close to $-\infty$ unless $\varphi(s) = \varphi_1(s)$ for all $s \le t$. By local uniqueness (proven by the contraction mapping method as above but starting with initial data given at a finite t), $\varphi(s) = \varphi_1(s)$ for all s.

To show that $\varphi(t) \in \Sigma_{\text{scat}}$ for each t, we fix t and compute:

$$\sup_r \|e^{-irA}\varphi(t)\| \le \sup_r \|e^{-irA}e^{-itA}\varphi_-\| + \int_{-\infty}^{t} \|e^{-iA(t+r-s)}J(\varphi(s))\|\, ds$$

$$\le \sup_r \|e^{-irA}\varphi_-\| + \beta \int_{-\infty}^{t} \|\varphi(s)\|_a^q \|\varphi(s)\|\, ds$$

$$\le \|\varphi_-\|_{\text{scat}} + \tfrac{1}{2}\eta_0$$

$$\sup_r \{(1+|r|)^d \|e^{-irA}\varphi(t)\|_a\}$$

$$\le \sup_r \{(1+|r|)^d \|e^{-i(t+r)A}\varphi_-\|_a\}$$

$$+ \sup_r \left\{(1+|r|)^d \int_{-\infty}^{t} \|e^{-iA(t+r-s)}J(\varphi(s))\|_a\, ds\right\}$$

$$\le \sup_r \{(1+|r|)^d (1+|t+r|)^{-d} \|\varphi_-\|_{\text{scat}}\}$$

$$+ \sup_r \left\{(1+|r|)^d \int_{-\infty}^{t} (1+|t+r-s|)^{-d}(1+|s|)^{-dq}\, ds\right\}$$

$$\times \beta c_2 (1+4\eta_0)(2\eta_0)^q$$

$$\le \sup_r \{(1+|r|)^d (1+|t+r|)^{-d}\}(\|\varphi_-\|_{\text{scat}} + \tfrac{1}{2}\eta_0)$$

Thus, $\varphi(t) \in \Sigma_{\text{scat}}$.

To prove (b), we estimate

$$\|\varphi(t) - e^{-itA}\varphi_-\| = \|e^{itA}\varphi(t) - \varphi_-\|$$

$$\le \int_{-\infty}^{t} \|e^{isA}J(\varphi(s))\|\, ds$$

$$\le \beta \int_{-\infty}^{t} \|\varphi(s)\|_a^q \|\varphi(s)\|\, ds$$

$$\le \beta(2\eta_0)^{q+1} \int_{-\infty}^{t} (1+|s|)^{-dq}\, ds$$

$$\to 0$$

as $t \to -\infty$. ∎

The solution of (255) constructed above satisfies (249b) with

$$\varphi_0 = \varphi_- + \int_{-\infty}^{0} e^{iAs}J(\varphi(s))\, ds$$

Part (a) of the following lemma completes the proof of Theorem XI.97. Part (b) is used in the proof of Theorem XI.100.

Lemma 1

(a) Suppose that $q \ge 1$, $d > 0$, and $dq > 1$. Then

$$\int_{-\infty}^{\infty} (1+|t-s|)^{-d}(1+|s|)^{-dq}\, ds \le c_3(1+|t|)^{-d}$$

(b) Suppose that $q > 1$, $d > 0$, and $dq > 1$. Then

$$\sup_r \left\{(1+|r|)^d \int_{t_1}^{t_2} (1+|r-s|)^{-d}(1+|s|)^{-dq}\, ds\right\} \to 0$$

as $t_1, t_2 \to +\infty$ or $t_1, t_2 \to -\infty$.

Proof (a) It is sufficient to consider the case where t is positive. We break the integral into two parts and estimate:

$$\int_{|s-t|\ge t/2} (1+|t-s|)^{-d}(1+|s|)^{-dq}\, ds$$

$$\le \left(1+\frac{t}{2}\right)^{-d} \int_{|s-t|\ge t/2} (1+|s|)^{-dq}\, ds$$

$$\le c(1+t)^{-d} \int_{-\infty}^{\infty} (1+|s|)^{-dq}\, ds$$

and for $d \ne 1$,

$$\int_{t/2}^{3t/2} (1+|t-s|)^{-d}(1+|s|)^{-dq}\, ds$$

$$\le \left(1+\frac{t}{2}\right)^{-dq} \left\{\int_{t/2}^{t} (1+(t-s))^{-d}\, ds + \int_{t}^{3t/2} (1+s-t)^{-d}\, ds\right\}$$

$$\le 2\left(1+\frac{t}{2}\right)^{-dq} \left\{|1-d|^{-1}\left(\left(1+\frac{t}{2}\right)^{-d+1} + 1\right)\right\}$$

$$\le c(1+t)^{-dq-d+1} + c(1+t)^{-dq}$$

$$\le c(1+t)^{-d}$$

since $dq > 1$ and $q \ge 1$.

If $d = 1$, the second integral can be estimated by

$$2\left(1 + \frac{t}{2}\right)^{-q} \ln\left(1 + \frac{t}{2}\right) \leq c(1 + t)^{-1}$$

since $q > 1$ if $d = 1$.

(b) Consider the case $t_2 > t_1 \to \infty$ and choose $q_0 \geq 1$ so that $dq_0 > 1$ and $q > q_0$. Then

$$(1 + |r|^d) \int_{t_1}^{t_2} (1 + |r - s|)^{-d}(1 + |s|)^{-dq}\, ds$$

$$\leq [(1 + |t_1|)^{-d(q-q_0)}](1 + |r|)^d \int_{-\infty}^{\infty} (1 + |r - s|)^{-d}(1 + |s|)^{-dq_0}\, ds$$

so (b) follows from (a). ∎

Theorem XI.98 (the scattering operator for small data) Assume all the hypotheses of Theorem XI.97 and let $\varphi(t)$ be the solution of (255) corresponding to $\varphi_- \in \Sigma_{\text{scat}}$ with $\|\varphi_-\|_{\text{scat}} \leq \eta_0$. Then, for η_0 sufficiently small:

(a) There exists $\varphi_+ \in \Sigma_{\text{scat}}$, with $\|\varphi_+\|_{\text{scat}} \leq 2\eta_0$, so that

$$\|\varphi(t) - e^{-itA}\varphi_+\| \to 0 \qquad \text{as} \quad t \to +\infty$$

(b) The map $\varphi_- \xrightarrow{S} \varphi_+$, defined on $\{\varphi \mid \|\varphi_-\|_{\text{scat}} < \eta_0\}$ is one-to-one and continuous in the $\|\cdot\|_{\text{scat}}$ norm.

Proof From Theorem XI.97 we know that $|||\varphi(\cdot)||| \leq 2\eta_0$. Thus

$$\|e^{it_1A}\varphi(t_1) - e^{it_2A}\varphi(t_2)\| \leq \left\| \int_{t_1}^{t_2} e^{isA} J(\varphi(s))\, ds \right\|$$

$$\leq \int_{t_1}^{t_2} \beta \|\varphi(s)\|_a^q \|\varphi(s)\|\, ds$$

$$\leq \beta(2\eta_0)^{q+1} \int_{t_1}^{t_2} (1 + |s|)^{-dq}\, ds$$

by (252). Thus $\{e^{itA}\varphi(t)\}$ is Cauchy in $\mathscr{H}$ as $t \to +\infty$ since $dq > 1$. Letting

$$\varphi_+ = \lim_{t \to +\infty} e^{itA}\varphi(t)$$

we have

$$\|\varphi(t) - e^{-itA}\varphi_+\| \to 0 \qquad \text{as} \quad t \to +\infty$$

by the unitarity of e^{-itA}. To show that $\varphi_+ \in \Sigma_{\text{scat}}$, observe that

$$e^{itA}\varphi(t) = \varphi_- + \int_{-\infty}^{t} e^{isA} J(\varphi(s))\, ds$$

Letting $t \to +\infty$, we conclude that

$$\varphi_+ = \varphi_- + \int_{-\infty}^{\infty} e^{isA} J(\varphi(s))\, ds$$

Now, by (254) and (252),

$$\|e^{-iA(t-s)}J(\varphi(s))\|_a \leq c_2(1 + |t - s|)^{-d}\{\|J(\varphi(s))\| + \|J(\varphi(s))\|_b\}$$

$$\leq c_2\beta(1 + |t - s|)^{-d}\{\|\varphi(s)\|_a^q(1 + 2\|\varphi(s)\|)\}$$

$$\leq c_2\beta(2\eta_0)^q(1 + 4\eta_0)(1 + |t - s|)^{-d}(1 + |s|)^{-dq}$$

for each s and t. Since

$$e^{-itA}\varphi_+ = e^{-itA}\varphi_- + \int_{-\infty}^{\infty} e^{-iA(t-s)} J(\varphi(s))\, ds$$

we conclude that $\|e^{-itA}\varphi_+\|_a < \infty$ and

$$\sup_t \{(1 + |t|)^d \|e^{-itA}\varphi_+\|_a\}$$

$$\leq \sup_t \{(1 + |t|)^d \|e^{-itA}\varphi_-\|_a\} + c_2\beta(2\eta_0)^q(1 + 4\eta_0)$$

$$\times \sup_t \left\{(1 + |t|)^d \int_{-\infty}^{\infty} (1 + |t - s|)^{-d}(1 + |s|)^{-dq}\, ds\right\}$$

$$\leq \sup_t (1 + |t|)^d \|e^{-itA}\varphi_-\|_a + \tfrac{1}{2}\eta_0$$

by the lemma (part a) and the choice of η_0 in Theorem XI.97. Thus

$$\|\varphi_+\|_{\text{scat}} \leq \|\varphi_-\|_{\text{scat}} + \tfrac{1}{2}\eta_0 + \tfrac{1}{2}\eta_0 \leq 2\eta_0$$

This proves (a).

To prove that S is continuous, let φ_- and ψ_- be in Σ_{scat} with $\|\varphi_-\|_{\text{scat}} \leq \eta_0$ and $\|\psi_-\|_{\text{scat}} \leq \eta_0$ and let $\varphi(t)$ and $\psi(t)$ be the corresponding solutions given by Theorem XI.97. We shall first show that $|||\varphi(\cdot) - \psi(\cdot)|||$ can be estimated by $\|\varphi_- - \psi_-\|_{\text{scat}}$ and then show that $\|\varphi_+ - \psi_+\|_{\text{scat}}$ can be estimated by $|||\varphi(\cdot) - \psi(\cdot)|||$. Since

$$\varphi(t) - \psi(t) = e^{-iAt}(\varphi_- - \psi_-) + \int_{-\infty}^{t} e^{-iA(t-s)}(J(\varphi(s)) - J(\psi(s)))\, ds$$

we have

$$\|\varphi(t) - \psi(t)\| \le \|\varphi_- - \psi_-\| + \int_{-\infty}^{t} \|J(\varphi(s)) - J(\psi(s))\|\, ds$$

$$\le \|\varphi_- - \psi_-\| + \beta(2\eta_0)^q \int_{-\infty}^{t} (1 + |s|)^{-dq} \|\varphi(s) - \psi(s)\|\, ds$$

$$\le \|\varphi_- - \psi_-\| + \beta(2\eta_0)^q \left(\int_{-\infty}^{\infty} (1 + |s|)^{-dq}\, ds \right) |||\varphi(\cdot) - \psi(\cdot)|||$$

Similarly,

$$\|\varphi(t) - \psi(t)\|_a$$

$$\le \|e^{-iAt}(\varphi_- - \psi_-)\|_a + \int_{-\infty}^{t} \|e^{-iA(t-s)}(J(\varphi(s)) - J(\psi(s)))\|_a\, ds$$

$$\le \|e^{-iAt}(\varphi_- - \psi_-)\|_a$$

$$+ c_2 \int_{-\infty}^{t} (1 + |t-s|)^{-d} \{ \|J(\varphi(s)) - J(\psi(s))\|_b + \|J(\varphi(s)) - J(\psi(s))\| \}\, ds$$

$$\le \|e^{-iAt}(\varphi_- - \psi_-)\|_a$$

$$+ 3c_2 \beta(2\eta_0)^q \left(\int_{-\infty}^{\infty} (1 + |t-s|)^{-d} (1 + |s|)^{-dq}\, ds \right) |||\varphi(\cdot) - \psi(\cdot)|||$$

Combining these two estimates, we have

$$|||\varphi(\cdot) - \psi(\cdot)||| \le \|\varphi_- - \psi_-\|_{\text{scat}} + c(\beta, \eta_0) |||\varphi(\cdot) - \psi(\cdot)|||$$

where

$$c(\beta, \eta_0) = \beta(2\eta_0)^q \int_{-\infty}^{\infty} (1 + |s|)^{-dq}\, ds$$

$$+ 3c_2 \beta(2\eta_0)^q \sup_t \left\{ (1 + |t|)^d \int_{-\infty}^{\infty} (1 + |t-s|)^{-d} (1 + |s|)^{-dq}\, ds \right\}$$

By choosing η_0 small enough, we can guarantee that $c(\beta, \eta_0) \le \frac{1}{2}$ implying that

$$|||\varphi(\cdot) - \psi(\cdot)||| \le 2\|\varphi_- - \psi_-\|_{\text{scat}} \tag{259}$$

Next

$$\|\varphi_+ - \psi_+\|_{\text{scat}} \le \|\varphi_- - \psi_-\|_{\text{scat}} + \left\| \int_{-\infty}^{\infty} e^{isA} (J(\varphi(s)) - J(\psi(s)))\, ds \right\|_{\text{scat}}$$

Using the usual estimates, we find that

$$\sup_t \left\| \int_{-\infty}^{\infty} e^{-iA(t-s)} (J(\varphi(s)) - J(\psi(s)))\, ds \right\| \le c(\beta, \eta_0) |||\varphi(\cdot) - \psi(\cdot)|||$$

and

$$\sup_t \left\{ (1 + |t|)^d \left\| \int_{-\infty}^{\infty} e^{-iA(t-s)} (J(\varphi(s)) - J(\psi(s)))\, ds \right\|_a \right\}$$

$$\le c(\beta, \eta_0) |||\varphi(\cdot) - \psi(\cdot)|||$$

so

$$\|\varphi_+ - \psi_+\|_{\text{scat}} \le \|\varphi_- - \psi_-\|_{\text{scat}} + c(\beta, \eta_0) |||\varphi(\cdot) - \psi(\cdot)|||$$

$$\le 2\|\varphi_- - \psi_-\|_{\text{scat}}$$

by (259) above. This proves that S is uniformly $\|\cdot\|_{\text{scat}}$ continuous for η_0 small enough. The proof that S is one-to-one is left to the reader (Problem 126). ∎

Before going on to examples, let us point out several important aspects of these theorems. First, the hypotheses do not require a priori estimates on the solution of the nonlinear equation, nor did we use energy inequalities. The only requirement was that solutions of the *linear* equation decay sufficiently rapidly and that the nonlinearity have high enough degree at zero. In particular, the verification of (i)–(iii) does not depend on the sign of the nonlinear term. Secondly, suppose that the nonlinear equation is of the form

$$\varphi'(t) = -iA\varphi(t) + \lambda J(\varphi(t)) \tag{260}$$

and (i)–(iii) hold. Then for any $\varphi_- \in \Sigma_{\text{scat}}$, the conclusions of Theorems XI.97 and XI.98 hold for λ small enough (the choice of λ depends on $\|\varphi_-\|_{\text{scat}}$). Finally, by slightly rearranging the proofs of the above theorems, we have global existence for the initial value problem at $t = 0$ if the data are small.

Theorem XI.99 Let A, $\mathscr{H}$, and J satisfy the hypotheses of Theorem XI.97. Then for η_0 small enough and any $\varphi_0 \in \Sigma_{\text{scat}}$ with $\|\varphi_0\|_{\text{scat}} \le \eta_0$, the

equation (249b) has a strongly continuous, global, Σ_{scat}-valued solution $\varphi(t)$ so that $\varphi(0) = \varphi_0$. Further, there exist φ_+, φ_- in Σ_{scat} so that

$$\|\varphi(t) - e^{-iAt}\varphi_+\| \to 0, \qquad t \to +\infty$$
$$\|\varphi(t) - e^{-iAt}\varphi_-\| \to 0, \qquad t \to -\infty$$

For any $\varphi_0 \in \Sigma_{\text{scat}}$, the same conclusion holds for the integral equation corresponding to (260) if λ is small enough (depending on $\|\varphi_0\|_{\text{scat}}$).

Example 1 (the nonlinear Schrödinger equation) We begin with an easy example, the nonlinear Schrödinger equation in one dimension,

$$\begin{aligned} iu_t &= -u_{xx} + \lambda|u|^{p-1}u \\ u(x, 0) &= f(x) \end{aligned} \tag{261}$$

because it illustrates nicely the method for choosing the norms described above. The corresponding free equation is

$$u_t - iu_{xx} = 0$$
$$u(x, 0) = f(x)$$

and $A = -d^2/dx^2$. The solution can be written explicitly as

$$u(x, t) = (4\pi it)^{-1/2} \int e^{i(x-y)^2/4t} f(y)\, dy$$

and thus

$$\|u(x, t)\|_\infty \le |t|^{-1/2}\|f\|_1$$

Therefore, we choose

$$\|u\|_a = \|u\|_\infty, \qquad \|u\|_b = \|u\|_1$$

We have thus satisfied hypothesis (ii) with $d = \frac{1}{2}$. Notice that we cannot choose $L^2(\mathbb{R})$ as our Hilbert space because it is not true that $\|u\|_\infty \le c\|u\|_2$. However, by the proof of Sobolev's lemma (Theorem IX.24):

$$\|u\|_\infty \le c\|Bu\|_2 \tag{262}$$

where as usual $B = \sqrt{-\Delta + m^2}$. Thus, we take

$$\|u\| = \|Bu\|_2$$

so that hypothesis (i) is satisfied. We must check for which p (iii) holds. In the following calculation we replace $|u|^{p-1}u$ by u^p, take p to be an integer, and treat B as though it were d/dx. By using the techniques of Lemmas 3–5 of Section X.13, one can easily handle the actual case. Letting P be a suitable polynomial, we have

$$\begin{aligned} \|J(u_1) - J(u_2)\| &= |\lambda|\,\|B(u_1^p - u_2^p)\|_2 \\ &= |\lambda|p\|(Bu_1)u_1^{p-1} - (Bu_2)u_2^{p-1}\|_2 \\ &\le |\lambda|p\|(Bu_1)(u_1 - u_2)P(u_1, u_2)\|_2 \\ &\quad + |\lambda|p\|(Bu_1 - Bu_2)u_2^{p-1}\|_2 \\ &\le C\|Bu_1\|_2\,\|u_1 - u_2\|_\infty\,\|P(u_1, u_2)\|_\infty \\ &\quad + C\|B(u_1 - u_2)\|_2\,\|u_2^{p-1}\|_\infty \\ &\le C\|Bu_1\|_2\,\|B(u_1 - u_2)\|_2(\|u_1\|_\infty + \|u_2\|_\infty)^{p-2} \\ &\quad + C\|B(u_1 - u_2)\|_2\,\|u_2\|_\infty^{p-1} \\ &\le \beta(\|u_1\|_a + \|u_2\|_a)^{p-2}\|u_1 - u_2\| \end{aligned}$$

for $\|u_1\|$ and $\|u_2\|$ small. Thus, the first hypothesis in (iii) holds with $q = p - 2$. Similarly,

$$\begin{aligned} \|J(u_1) - J(u_2)\|_b &= \|u_1^p - u_2^p\|_1 \\ &= \|(u_1 - u_2)Q(u_1, u_2)\|_1 \\ &\le C\|B(u_1 - u_2)\|_2(\|u_1\|_2 + \|u_2\|_2)(\|u_1\|_\infty + \|u_2\|_\infty)^{p-2} \\ &\le \beta\|u_1 - u_2\|(\|u_1\|_\infty + \|u_2\|_\infty)^{p-2} \end{aligned}$$

for $\|u_1\|$ and $\|u_2\|$ small, so the second part of (iii) also holds with $q = p - 2$. Now, since $d = \frac{1}{2}$ and we need $dq > 1$, we must require $q > 2$. Therefore if $p > 4$, Theorems XI.97–XI.99 provide small data global existence and a scattering theory for equation (261).

Example 2 (the nonlinear Klein–Gordon equation, $n = 1$) In order to discuss the equation

$$u_{tt} - u_{xx} + m^2u = -\lambda u^p \tag{263}$$

we first need a decay estimate for the linear equation

$$\begin{aligned} u_{tt} - u_{xx} + m^2u &= 0 \\ u(x, 0) &= f \\ u_t(x, 0) &= g \end{aligned} \tag{264}$$

in terms of tractable norms on the initial data. Thus stationary phase methods are not enough, and we shall have to use the explicit formula for the solution of the linear equation in terms of special functions.

Lemma 2 Suppose that f and g are in $\mathscr{S}(\mathbb{R})$ and let $u(x, t)$ be the solution of (264) with initial data $\langle f, g\rangle$. Then

$$\|u(x, t)\|_\infty \le C|t|^{-1/2}\{\|f\|_1 + \|f'\|_1 + \|f''\|_1 + \|g'\|_1 + \|g\|_1\} \quad (265)$$

Proof For each t, let $u(t)$ denote $u(\cdot, t)$ as an $L^2(\mathbb{R}^3)$-valued function. $u(t)$ is given by

$$u(t) = \cos(Bt)f + \frac{\sin(Bt)}{B}g$$

or

$$[\widehat{u(t)}](k) = \cos(t\sqrt{k^2+m^2})\hat{f}(k) + \frac{\sin(t\sqrt{k^2+m^2})}{\sqrt{k^2+m^2}}\hat{g}(k)$$

Thus $u(t)$ can be written

$$u(t) = \frac{\partial R}{\partial t} * f + R * g$$

where for each t, R is the inverse Fourier transform

$$R(x, t) = (2\pi)^{-1}\int_{-\infty}^{\infty} e^{ikx}\frac{\sin t\sqrt{k^2+m^2}}{\sqrt{k^2+m^2}}\,dk$$

in the sense of distributions. The convolution $R * g$ makes sense since $R \in \mathscr{S}'(\mathbb{R})$ and $g \in \mathscr{S}(\mathbb{R})$. There are many ways to figure out what the function $R(x, t)$ is. Here is one. First we notice that $R(x, t)$ is zero except when $x^2 \le t^2$. This follows from the Paley–Wiener theorem for distributions and the analyticity and growth of $(k^2+m^2)^{-1/2}\sin t\sqrt{k^2+m^2}$ in the imaginary k directions. Secondly, we can compute directly that $R(x, t)$ is invariant under two-dimensional Lorentz transformations. Thus for $t > 0$, $R(x, t)$ is a function of $t^2 - x^2$. Suppose that we write for $x^2 \le t^2$, $t > 0$,

$$H(\sqrt{t^2-x^2}) \equiv R(x, t) = (2\pi)^{-1}\int_{-\infty}^{\infty} e^{ikx}\frac{\sin t\sqrt{k^2+m^2}}{\sqrt{k^2+m^2}}\,dk$$

Then, differentiating twice with respect to t and twice with respect to x and subtracting the results, one finds that H satisfies

$$H''(y) + \frac{1}{y}H'(y) + m^2H(y) = 0$$

so

$$H(y) = cJ_0(my) + dY_0(my)$$

where J_0 and Y_0 are Bessel functions. d must be zero since $R(\cdot, t) \in L^2(\mathbb{R})$ and Y_0 has a $1/y$ singularity at $y = 0$. Setting $x = 0$, one determines that $c = \frac{1}{2}$. Thus, for $t > 0$,

$$R(x, t) = \tfrac{1}{2}\chi_{\{x|x^2\le t^2\}}(x)J_0(m\sqrt{t^2-x^2})$$

Therefore we have the representation

$$(R * g)(x, t) = \tfrac{1}{2}\int_{-t}^{t} J_0(m\sqrt{t^2-y^2})g(x-y)\,dy \quad (266)$$

To analyze the decay of $R * g$ we need the estimates

$$J_0(\mu) = \left(\frac{2}{\mu\pi}\right)^{\frac{1}{2}}\cos\left(\mu - \frac{\pi}{4}\right) + O(\mu^{-\frac{1}{2}})$$

$$J_1(\mu) = O(\mu^{-\frac{1}{2}})$$

as $\mu \to \infty$. We write (266) as an integral over $\{y\,|\,|y| \le \frac{1}{2}t\}$ and an integral over $\{y\,|\,\frac{1}{2}t \le |y| \le t\}$. Using $|J_0(\mu)| \le c\mu^{-1/2}$, the first can easily be estimated by

$$ct^{-1/2}\int_{-\frac{1}{2}t}^{\frac{1}{2}t}|g(x-y)|\,dy \le ct^{-1/2}\|g\|_1 \quad (267)$$

There are two integrals left, one of which is

$$\tfrac{1}{2}\int_{\frac{1}{2}t}^{t} J_0(m\sqrt{t^2-y^2})g(x-y)\,dy$$

$$= \left(\frac{1}{2\pi m}\right)^{1/2}\int_{\frac{1}{2}t}^{t}\frac{\cos(m\sqrt{t^2-y^2}-\frac{1}{4}\pi)}{(t^2-y^2)^{1/4}}g(x-y)\,dy$$

$$+ \int_{\frac{1}{2}t}^{t} O((t^2-y^2)^{-3/4})g(x-y)\,dy$$

For the second term, we have

$$\int_{\frac{1}{2}t}^{t} O((t^2-y^2)^{-3/4})g(x-y)\,dy \le ct^{-3/4}\|g\|_\infty\int_{\frac{1}{2}t}^{t}(t-y)^{-3/4}\,dy$$

$$\le ct^{-1/2}\|g\|_\infty$$

To handle the first term, we integrate by parts obtaining:

$$-g(x-y)\frac{(t^2-y^2)^{1/4}}{my\sqrt{2\pi m}}\sin\left(m\sqrt{t^2-y^2}-\frac{\pi}{4}\right)\Bigg]_{y=\frac{1}{2}t}^{y=t}$$
$$+\frac{1}{m\sqrt{2\pi m}}\int_{\frac{1}{2}t}^{t}\sin\left(m\sqrt{t^2-y^2}-\frac{\pi}{4}\right)\frac{d}{dy}\left\{\frac{(t^2-y^2)^{1/4}}{y}g(x-y)\right\}dy$$

Both terms may be easily estimated by $ct^{-1/2}(\|g\|_1+\|g'\|_1)$. Combining this with (267), we have

$$\|R*g\|_\infty \le ct^{-1/2}(\|g\|_1+\|g'\|_1)$$

To treat the $(\partial R/\partial t)*f$ term, notice that

$$\frac{\partial R}{\partial t}=\frac{1}{2}(\delta(x+t)+\delta(x-t))+\frac{1}{2}m\frac{t}{\sqrt{t^2-x^2}}J_1(m\sqrt{t^2-x^2})$$

so

$$\left(\frac{\partial R}{\partial t}*f\right)(x,t)=\frac{1}{2}\{f(x+t)+f(x-t)\}$$
$$+\frac{1}{2}m\int_{-t}^{t}\frac{t}{\sqrt{t^2-y^2}}J_1(m\sqrt{t^2-y^2})f(x-y)\,dy \quad (268)$$

First we estimate the integral over $\{y\,|\,|y|\le\frac{1}{2}t\}$ as before. Then we integrate the remaining integral by parts, observe that the boundary terms at $y=\pm t$ cancel the first term in (268), and estimate the other boundary terms and the remaining integral by a second integration by parts just as we did for $R*g$. The result is

$$\left\|\left(\frac{\partial R}{\partial t}*f\right)\right\|_\infty \le ct^{-1/2}(\|f\|_1+\|f'\|_1+\|f''\|_1)$$

The extra derivative on f occurs because there was one extra integration by parts. This proves the lemma. ∎

For f and g nice, this lemma gives us a decay estimate and leads us to define

$$\|\langle u,v\rangle\|_a=\|u\|_\infty$$
$$\|\langle u,v\rangle\|_b=\|u\|_1+\|u'\|_1+\|u''\|_1+\|v\|_1+\|v'\|_1$$

We take as our Hilbert space

$$\mathscr{H}=\left\{\varphi=\langle u,v\rangle\;\middle|\;\|\varphi\|^2=\|Bu\|_2^2+\|v\|_2^2<\infty\right\}$$

Then, by (262), (i) holds. By the lemma,

$$\|e^{-itA}\varphi\|_a\le c|t|^{-1/2}\|\varphi\|_b$$

for nice φ. By the linearity, this extends to all $\varphi\in\mathscr{H}$. Thus we have (ii). It remains to check for which p (iii) holds. Since $J(\varphi)=\langle 0,-\lambda u^p\rangle$,

$$\|J(\varphi_1)-J(\varphi_2)\|\le|\lambda|\,\|u_1^p-u_2^p\|_2$$
$$\le c|\lambda|\,\|u_1-u_2\|_2(\|u_1\|_\infty+\|u_2\|_\infty)^{p-1}$$
$$\le c|\lambda|(\|\varphi_1\|_a+\|\varphi_2\|_a)^{p-1}\|\varphi_1-\varphi_2\|$$
$$\|J(\varphi_1)-J(\varphi_2)\|_b=|\lambda|\{\|u_1^p-u_2^p\|_1+\|(u_1^p-u_2^p)'\|_1\}$$
$$\le c|\lambda|\{\|u_1-u_2\|_2+\|u_1'-u_2'\|_2\}$$
$$\times(\|u_1\|_2+\|u_2\|_2)(\|u_1\|_\infty+\|u_2\|_\infty)^{p-2}$$
$$\le|\lambda|(\|\varphi_1\|_a+\|\varphi_2\|_a)^{p-2}\|\varphi_1-\varphi_2\|$$

Thus, the estimates in hypothesis (iii) are satisfied with $q=p-2$. Since $d=\frac{1}{2}$ and we need $dq>1$, we must choose $q>2$ so $p>4$. We have thus proven, by Theorems XI.97–XI.99, global existence for small Cauchy data and the existence of the scattering operator for small data if $p>4$. Notice that this result holds whatever the sign of λ and whether p is either even or odd (or fractional).

Example 3 (nonlinear Klein–Gordon equation, $n=3$) In order to handle the nonlinear Klein–Gordon equation (245) with $F(u)=-\lambda|u|^{p-1}u$ in three dimensions we first need a lemma which is analogous to Lemma 2.

Lemma 3 Let $f,g\in\mathscr{S}(\mathbb{R}^3)$ and let $u(x,t)$ be the solution of

$$u_{tt}-\Delta u+m^2u=0$$
$$u(x,0)=f(x)$$
$$u_t(x,0)=g(x)$$

Then, there is a universal constant c so that

$$\|u(x,t)\|_\infty\le c|t|^{-3/2}\|\langle f,g\rangle\|_b \quad (269)$$

where $\|\langle f,g\rangle\|_b$ is defined as the sum of the L_1 norms of all the derivatives of f of order ≤ 3 and all the derivatives of g of order ≤ 2.

The proof of this lemma is similar to the proof of Lemma 2; only the determination of the form of $R(x, t)$ is a little more complicated. The extra derivative on the initial data comes about because $R(x, t)$ itself involves J_1. Thus, one must integrate by parts twice for the g terms and three times for the f terms. We spare the reader the details.

So, we choose $\|\varphi\|_b$ to be as defined in the lemma and $\|\varphi\|_a = \|u\|_\infty$. Then, (ii) is satisfied with $d = \frac{3}{2}$. However, we can no longer use the Hilbert space $\mathscr{H}$ because it is not true that $\|u\|_\infty \le c\|Bu\|_2$ in three dimensions. It *is* true that $\|u\|_\infty \le c\|B^2u\|_2$, so we can use

$$\|\langle u, v\rangle\|^2 = \|B^2u\|_2^2 + \|Bv\|_2^2$$

$$\mathscr{H}_1 = \left\{ \langle u, v\rangle \,\middle|\, \|\langle u, v\rangle\| < \infty \right\}$$

Then, the free dynamics is unitary on $\mathscr{H}_1$ and (i) holds. Further, similar calculations to those in one dimension show that

$$\begin{aligned}\|J(\varphi_1) - J(\varphi_2)\| &= |\lambda|\,\|B(u_1^p - u_2^p)\|_2 \\ &\le |\lambda|(\|\varphi_1\| + \|\varphi_2\|)(\|\varphi_1\|_a + \|\varphi_2\|_a)^{p-2}\|\varphi_1 - \varphi_2\|\end{aligned}$$

There are many terms in $\|J(\varphi_1) - J(\varphi_2)\|_b$. Let us look at one of highest order in D (denote by D_i any partial derivative):

$$\begin{aligned}&\|D_i^2(u_1^p - u_2^p)\|_1 \\ &\quad\le \|(D_i^2(u_1 - u_2))P(u_1, u_2)\|_1 + 2\|(D_i(u_1 - u_2))D_iP(u_1, u_2)\|_1 \\ &\qquad + \|(u_1 - u_2)D_i^2P(u_1, u_2)\|_1 \\ &\quad\le C(\|Bu_1\|_2 + \|Bu_2\|_2)(\|u_1\|_\infty + \|u_2\|_\infty)^{p-2}\|B^2(u_1 - u_2)\|_2 \\ &\qquad + C(\|Bu_1\|_2 + \|Bu_2\|_2)^2(\|u_1\|_\infty + \|u_2\|_\infty)^{p-3}\|u_1 - u_2\|_\infty \\ &\quad\le \beta\{(\|\varphi_1\|_a + \|\varphi_2\|_a)^{p-3}\|\varphi_1 - \varphi_2\|_a + (\|\varphi_1\|_a + \|\varphi_2\|_a)^{p-2}\|\varphi_1 - \varphi_2\|\}\end{aligned}$$

Thus, (iii) is satisfied with $q = p - 2$ for slightly different reasons than in one dimension (you should not assume that $q = p - 2$ is all right in all dimensions). Notice in the case $q = 1$, the constant β in (iii) is small if $\|\varphi_1\| + \|\varphi_2\|$ is small. Since $d = \frac{3}{2}$, we need only choose $q \ge 1$, so $p \ge 3$. For all such p, we have a scattering theory and global existence for the equation

$$u_{tt} - \Delta u + m^2u = -\lambda|u|^{p-1}u, \qquad x \in \mathbb{R}^3 \tag{270}$$

for small data independent of whether p is even or odd and of the sign of λ.

In order to discuss scattering for solutions of nonlinear equations where neither the data nor the coupling constant is small one needs global existence results. Thus, unlike the case of small data, the nonlinear terms usually have to have the right signs so that there is a conserved energy that is bounded below. Using such a conserved quantity, one shows that the norm of any local solution cannot go to infinity in finite time and thus that global solutions exist (see Section X.13). If we have global existence, then we can construct the wave operators by methods similar to those that we used in the case of small data. In the following we denote by M_t the group of *nonlinear* operators

$$M_t\colon \varphi_0 \to \varphi(t)$$

where $\varphi(t)$ solves

$$\varphi(t) = e^{-itA}\varphi_0 + \int_0^t e^{-iA(t-s)}J(\varphi(s))\,ds \tag{249b}$$

Theorem XI.100 (existence of the wave operators) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J a nonlinear mapping of $\mathscr{H}$ into itself. Suppose that there exist norms $\|\cdot\|_a$, $\|\cdot\|_b$ so that the hypotheses (i)–(iii) hold with $q > 1$. Suppose that for each η and T, the solutions $M_t\varphi_0$ of (249b) are uniformly bounded (in $\|\cdot\|$-norm) for all $\|\varphi_0\| \le \eta$ and all $0 < |t| \le T$. Then:

(a) For each $\varphi_- \in \Sigma_{\text{scat}}$, there is a unique global solution $\varphi(\cdot)$ of (249b) so that $\varphi(t) \in \Sigma_{\text{scat}}$ for each t, and

$$\|\varphi(t) - e^{-iAt}\varphi_-\| \to 0 \qquad \text{as} \quad t \to -\infty$$

(b) The mapping $\Omega^+\colon \varphi_- \to \varphi(0)$ is a one-to-one map of Σ_{scat} into Σ_{scat} that is uniformly continuous on balls in Σ_{scat}.

(c) Analogous statements as in (a) and (b) hold for $\varphi_+ \in \Sigma_{\text{scat}}$, $t \to +\infty$, and the map $\Omega^-\colon \varphi_+ \to \varphi(0)$.

Proof We just sketch the proof since the details are very similar to the case of small data. Let $\varphi_- \in \Sigma_{\text{scat}}$ be given, $\|\varphi_-\|_{\text{scat}} \le \eta$ (note that η is not assumed small). Let $X_{\eta,\varphi_-,T}$ denote the $\mathscr{H}$-valued continuous functions $\psi(\cdot)$ on $(-\infty, T]$ so that

$$\begin{aligned}&|||\psi(t) - e^{-itA}\varphi_-|||_{(-\infty,T]} \\ &\quad\equiv \sup_{-\infty \le t \le T}\|\psi(t) - e^{-itA}\varphi_-\| + \sup_{-\infty \le t \le T}(1 + |t|)^d\|\psi(t) - e^{-itA}\varphi_-\|_a \\ &\quad\le \eta\end{aligned}$$

For each T, $X_{\eta,\varphi_-,T}$ is a complete metric space. We define $\mathscr{J}$ and $\mathscr{M}$ as before so that

$$(\mathscr{M}\psi)(t) = e^{-iAt}\varphi_- + (\mathscr{J}\psi)(t)$$

The estimates (256) and (257) of Theorem XI.97 show that $\|\|(\mathscr{J}\psi)(t)\|\|_{(-\infty,T)}$ is small and that $\mathscr{M}$ is a contraction so long as T is sufficiently close to $-\infty$. (Since the data are not small, the smallness must come from part (b) of Lemma 1, which is why we require $q > 1$.) Thus $\mathscr{M}$ has a fixed point in X_{η,φ_-,T_0} for some fixed T_0. Just as in Theorem XI.97, one can prove that $\varphi(t) \in \Sigma_{\text{scat}}$ for each $t \in (-\infty, T_0]$ and that the limits in (a) hold.

By the estimates (256) and (257), we can use the same T_0 for all φ_- with $\|\varphi_-\| \leq \eta$. Thus, we can define the map

$$\Omega^+_{T_0}\colon \varphi_- \mapsto \varphi(T_0)$$

on $\mathscr{B}_\eta \equiv \{\psi \in \Sigma_{\text{scat}} \mid \|\psi\|_{\text{scat}} \leq \eta\}$ and as in Theorems XI.97 and XI.98, $\Omega^+_{T_0}$ is a one-to-one uniformly continuous map of $\mathscr{B}_\eta$ into Σ_{scat}. Thus far, global existence has not been used.

It can easily be checked that for $t \leq T_0$ our solution $\varphi(t)$ satisfies

$$\varphi(t) = e^{-iA(t-T_0)}\varphi(T_0) + \int_{T_0}^{t} e^{-iA(t-s)}J(\varphi(s))\,ds$$

Since J is Lipschitz, this equation can be solved locally in a neighborhood of T_0 by $\varphi(t) = M_{t-T_0}\varphi(T_0)$; by the boundedness hypothesis on M_t, this solution is global in t. By local uniqueness this definition of $\varphi(t)$ coincides with the $\varphi(t)$ defined earlier for $t \leq T_0$. It is easy to check that $\varphi(t)$ satisfies (249b) and that (254) and (253) imply that $\varphi(t)$ is in Σ_{scat} for all t. In fact, the uniform boundedness of M_t assumed in the hypotheses combined with (253) and (254) imply that for each t and each η_0, M_t is a uniformly continuous one-to-one map of $\mathscr{B}_{\eta_0}$ into Σ_{scat} (Problem 128). Thus, for each η, we define

$$\Omega^+ = M_{-T_0}\Omega^+_{T_0}$$

that is,

$$\Omega^+\colon \varphi_- \to \varphi(0)$$

We note that T_0 depends on η. By the properties of M_{-T_0} and $\Omega^+_{T_0(\eta)}$, we have that Ω^+ is a one-to-one uniformly continuous map of $\mathscr{B}_\eta$ into Σ_{scat}. Since η was arbitrary, Ω^+ takes Σ_{scat} into Σ_{scat} and is uniformly continuous on balls. An easy argument shows that Ω^+ is one-to-one on all of Σ_{scat}. This proves (a) and (b); the proof of (c) is similar. ∎

Examples 1 and 2, revisited To prove existence of the wave operators we need just check global existence and uniform continuity. For the nonlinear Klein–Gordon equation, this was done for $\lambda > 0, p \geq 1$ in Problem 75 of Chapter X. Similar methods (Problem 130) work for the nonlinear Schrödinger equations, using the Hilbert space of Example 1 and the conserved quantities

$$\int_{\mathbb{R}} |u(x,t)|^2\,dx, \qquad \int_{\mathbb{R}} \frac{1}{2}|u_x(x,t)|^2 + \frac{1}{p+1}|u(x,t)|^{p+1}\,dx$$

Thus, by Theorem XI.100 and the analysis of Examples 1 and 2, the wave operators exist if $p > 4$ and $\lambda > 0$.

Example 3, revisited For the case $n = 3$, we computed in Example 3 that the hypotheses (i)–(iii) hold with $d = \frac{3}{2}$ and $q = p - 2$. Since we must have $q > 1$ in Theorem XI.100, we must take $p > 3$. For $p \geq 5$, the global existence of strong solutions to (270) is open; For $p = 3$, the methods of Section X.13 give global existence and uniform continuity on balls. For the borderline case $p = 3$, one can get around the fact that Theorem XI.100 does not hold when $q = 1$ by using the following special estimates:

$$\begin{aligned}\|e^{-iA(t-s)}J(\varphi(s))\|_a &= \|B^{-1}\sin[(t-s)B]u^3(s)\|_\infty \\ &\leq C\|Bu^3(s)\|_2 \\ &\leq C\|\varphi(s)\|\,\|\varphi(s)\|_a^2\end{aligned}$$

With this estimate the proof of Theorem XI.100 goes through in the case $p = 3$. The reader is asked to provide the details in Problem 129.

This illustrates a very important point. Since the hypotheses of Theorems XI.97–XI.101 and techniques of proof are quite general, one can often do better in specific applications by using special properties of the particular operators at hand.

As in the quantum-mechanical case, we have now arrived at a really hard problem, the question of asymptotic completeness. To see what is involved let φ_0 be in the range of the Ω^+ constructed in Theorem XI.100. What we must show is that there is a φ_+ so that the solution $\varphi(t)$ of

$$\varphi(t) = e^{-itA}\varphi_0 + \int_0^t e^{-iA(t-s)}J(\varphi(s))\,ds$$

satisfies

$$\|\varphi(t) - e^{-itA}\varphi_+\| \to 0 \qquad \text{as} \quad t \to +\infty$$

By Cook's method, we should try to construct φ_+ by showing that $e^{itA}\varphi(t)$ is Cauchy in t as $t \to \infty$. Using (249b),

$$\|e^{it_1A}\varphi(t_1) - e^{it_2A}\varphi(t_2)\| \leq \int_{t_2}^{t_1} \|J(\varphi(s))\|\, ds$$

So, what we need is

$$\int_{-\infty}^{\infty} \|J(\varphi(s))\|\, ds < \infty \tag{270a}$$

Typically, in order to prove (270a) one needs to prove a priori estimates which guarantee that all solutions of (249) with nice initial data decay sufficiently rapidly in t in appropriate norms. Furthermore, to prove continuity of the scattering operator, the constants in this decay must be estimated in terms of the decay of the corresponding solution of the free equation. As we explained at the beginning of this section, such decay will not hold for general nonlinear equations because of the possibility of bound states. But even when the equation has no bound states, proving an a priori estimate is very difficult. Indeed, only very special cases have been treated. We will indicate the techniques involved by proving:

Theorem XI.101 Let f and g be real-valued functions in $C_0^\infty(\mathbb{R}^3)$ and let u denote the solution of

$$\begin{aligned} u_{tt} - \Delta u &= -u^3, \qquad x \in \mathbb{R}^3, \quad t \in \mathbb{R} \\ u(x, 0) &= f(x), \qquad u_t(x, 0) = g(x) \end{aligned} \tag{270b}$$

Let $\varphi(t) = \langle u(x, t), u_t(x, t)\rangle$ and let $\|\varphi\|$ denote the free energy norm, $\|\varphi\|^2 = \|\nabla u\|_2^2 + \|u_t\|_2^2$. Let e^{-itA}, where $A = i\left[\begin{smallmatrix} 0 & I \\ \Delta & 0 \end{smallmatrix}\right]$, be the group corresponding to solutions of the free wave equation $v_{tt} - \Delta v = 0$. Then there exist $\psi_\pm$, satisfying $\|\psi_\pm\| < \infty$, such that $\|\varphi(t) - e^{-itA}\psi_\pm\| \to 0$, as $t \to \pm\infty$.

The existence of smooth solutions of (270b) is discussed in Problem 76 of Chapter X. Using the methods of Section X.13 one can prove that if the initial data are in $C_0^\infty \times C_0^\infty$, then $u(x, t)$ will be in $C_0^\infty \times C_0^\infty$ for all t. Results similar to those in Theorem XI.101 hold for complex-valued solutions if $-u^3$ is replaced by $-u|u|^2$. Theorem XI.101 is not completely satisfactory. Although it does show that solutions of (270b) with nice initial data are asymptotically free, it does not say which $\psi_\pm$ do occur. Thus, we do not have an explicit domain for the scattering operator. Nevertheless, the proof of Theorem XI.101 will illustrate the difficulties that need to be overcome in proving asymptotic completeness results.

Our proof of Theorem XI.101 will rely on the existence of a special conserved quantity, the **conformal charge**,

$$Q_C = \int k_0(\mathbf{x}, t)\, d^3x \tag{270c}$$

where

$$k_0(x, t) = (t^2 + |\mathbf{x}|^2)[\tfrac{1}{2}u_t^2 + \tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{4}u^4] + 2tu_t\,\mathbf{x}\cdot\nabla u + 2tu_t u - u^2 \tag{270d}$$

Using the fact that u satisfies (270b) and has compact support for each t, one can check that Q_C is independent of t. The answer to the more subtle question, How does one find such conserved quantities?, is described in the appendix. In addition, the procedure explains which terms have to be integrated by parts to verify the independence.

Proof of Theorem XI.101 Since $J\langle u, v\rangle = \langle 0, -u^3\rangle$, we have that $\|J(\varphi(s))\| = \|u^3\|_2$. Using the fact that the energy

$$E(t) = \int [\tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{2}u_t^2 + \tfrac{1}{4}u^4]\, d^3x$$

is conserved and the Sobolev estimate $\|u\|_6 \leq C\|\sqrt{-\Delta + 1}\,u\|_2$, it follows easily (see Problem 76 in Chapter X) that $\|u(s)^3\|_2$ is bounded as s runs through any compact set. Thus in order to prove that (270a) holds, we must just show that $\|u(s)^3\|_2$ decays sufficiently rapidly at ∞. Writing $\|u(s)^3\|_2 \leq \|u(s)\|_\infty \|u(s)^2\|_2$, we shall first use the fact that Q_C is conserved to show that $\|u(s)^2\|_2 \leq C|s|^{-1}$ and then use, in addition, a Sobolev estimate and iteration to show that $\|u(s)\|_\infty \leq C|s|^{-1/6}$.

We begin by noting that

$$r^{-1}\nabla(ru) = \nabla u + r^{-2}\mathbf{r}u$$

so that

$$(r^2 + t^2)(\nabla u)^2 = (r^2 + t^2)[r^{-1}\nabla(ru)]^2 + r^{-2}(r^2 + t^2)u^2 + A$$

where

$$A = -2u\frac{\partial(ru)}{\partial r} - 2r^{-2}t^2u\frac{\partial(ru)}{\partial r}$$

After some manipulation, one finds that

$$r^2A = r^2u^2 - t^2u^2 - \frac{\partial}{\partial r}(r^3u^2 + t^2ru^2)$$

so

$$\int_{\mathbb{R}^3} A\, d^3x = \int_{\mathbb{R}^3} u^2 r^{-2}(r^2 - t^2)\, d^3x$$

since $\int r^{-2}(\partial f/\partial r)\, d^3x = -4\pi f(0)$ if f has compact support, is smooth away from zero, and C^1 up to zero. We conclude that

$$\int (r^2 + t^2)(\nabla u)^2\, d^3x = \int [(r^2 + t^2)(r^{-1}\nabla(ru))^2 + 2u^2]\, d^3x$$

so

$$Q_C = \int (t^2 + |x|)^2(\tfrac{1}{4}u^4)\, d^3x + \int B\, d^3x$$

where

$$B = \tfrac{1}{2}(r^2 + t^2)[(r^{-1}\nabla(ru))^2 + u_t^2] + 2tu_t\, \mathbf{x} \cdot (r^{-1}\nabla(ru))$$

Using $abcd \le [\frac{1}{2}(a^2 + c^2)][\frac{1}{2}(b^2 + d^2)]$, we see that B is positive, so $\int u^4\, d^3x \le 4Q_C t^{-2}$, which yields

$$\|u(t)^2\|_2 \le C|t|^{-1} \tag{270e}$$

Let $\varphi_0 = \langle f, g\rangle$. The first component of $e^{-itA}\langle f, g\rangle$ satisfies the free wave equation and, by (216a), may be represented by

$$[e^{-itA}\langle f, g\rangle]_1 = (4\pi t)^{-1} \int g(x + y)\, dS_{|t|} + \frac{d}{dt}\left[(4\pi t)^{-1} \int f(x + y)\, dS_{|t|}\right]$$

where $dS_{|t|}$ is the usual measure on the sphere of radius $|t|$ (with center at 0), normalized so that $\int dS_{|t|} = 4\pi t^2$. From this explicit representation it immediately follows that, for $f, g \in C_0^\infty(\mathbb{R}^3)$,

$$\|[e^{-itA}\varphi_0]_1\|_\infty \le C(1 + |t|)^{-1} \tag{270f}$$

Moreover,

$$\|[e^{-itA}\langle 0, g\rangle]_1\|_\infty \le C|t|^{-1/2}\|\nabla g\|_{6/5} \tag{270g}$$

To prove this we let $|y| = 1$, $t > 0$, and write

$$|g(y)| \le \int_1^\infty |(\nabla g)(ry)|\, dr$$

so, by Hölder's inequality,

$$\left|\int g(y)\, dS_1\right| \le \int_{S_1}\int_1^\infty (|\nabla g|r^{5/3})r^{-5/3}\, dr\, dS_1$$
$$\le C\left\{\int_{S_1}\int_1^\infty |\nabla g|^{6/5}r^2\, dr\, dS_1\right\}^{5/6}$$

where $C = (4\pi \int_1^\infty r^{-10}\, dr)^{1/6} < \infty$. This estimate and scaling imply (for $t > 0$):

$$\left|\frac{1}{4\pi t}\int_{S_t} g(x + y)\, dS_t\right| \le Ct^{-1/2}\left\{\int_{S_1}\int_t^\infty |\nabla g|^{6/5}r^2\, dr\, dS_1\right\}^{5/6}$$

which yields (270g).

Now, suppose that u solves (270b). Then (270f) and (270g) imply (for $t > 0$):

$$\|u(\cdot, t)\|_\infty \le \|[e^{-itA}\varphi_0]_1\|_\infty + \int_0^t \|[e^{-i(t-s)A}\langle 0, -u(s)^3\rangle]_1\|_\infty\, ds$$
$$\le C(1 + t)^{-1} + C\int_0^t (t - s)^{-1/2}\|\nabla(u(s)^3)\|_{6/5}\, ds$$

Using (270e) and the fact that $\|\nabla u\|_2$ is a priori bounded by the conservation of energy,

$$\|\nabla u^3\|_{6/5} \le 3\|(\nabla u)u^2\|_{6/5} \le 3\|\nabla u\|_2\|u^2\|_3$$
$$\le C\|u\|_4^{4/3}\|u\|_\infty^{2/3}$$
$$\le C(1 + s)^{-2/3}\|u\|_\infty^{2/3}$$

Thus, if we let $M(t) \equiv \sup_{0\le s\le t}\|u(\cdot, s)\|_\infty$, we have

$$\|u(\cdot, t)\|_\infty \le C(1 + t)^{-1} + DM(t)^{2/3}t^{-1/6}$$

where $D = C\int_0^1 (1 - \sigma)^{-1/2}\sigma^{-2/3}\, d\sigma < \infty$. From this we first conclude that $\sup_{0\le t<\infty} M(t) < \infty$ and then that

$$\|u(\cdot, t)\|_\infty \le C|t|^{-1/6} \tag{270h}$$

for $t > 0$. The proof for $t < 0$ is similar. (270h) and (270e) imply (270a) and, as indicated above, (270a) implies the result of the theorem. ∎

Appendix to Section XI.13: Conserved currents

One way to see that Q_C, given by (270c), is conserved is to observe that if we define

$$\mathbf{k} = -(\nabla u)\{(|\mathbf{x}|^2 + t^2)u_t + 2t\mathbf{x}\cdot\nabla u + 2tu\} - 2t\mathbf{x}(\tfrac{1}{2}u_t^2 - \tfrac{1}{2}(\nabla u)^2 - \tfrac{1}{4}u^4) \tag{270i}$$

and use the differential equation (270b), then we can compute that

$$\frac{\partial k_0}{\partial t} + \nabla\cdot\mathbf{k} = 0$$

Thus,

$$\frac{d}{dt}Q_C = \int \frac{\partial k_0}{\partial t}\, d^3x = -\int \nabla\cdot\mathbf{k}\, d^3x = 0$$

where we have used the fact that u, and therefore $\mathbf{k}$, is C^∞ with compact support in x for each t (this follows from the fact that the initial data are in $C_0^\infty(\mathbb{R}^3)$).

The group of ideas, generally called Noether's theorem, which explains how to find such k_0 and $\mathbf{k}$ are the subject of this appendix. They are best described by a Lagrangian formalism which we introduce first. Let $\mathbf{x}$ be in $\mathbb{R}^n$ and u a real-valued function of $\mathbf{x}$ (for the extension to multicomponent u, see Problem 152). Let $\mathscr{L}$ be a function of $n+2$ real variables $\mathscr{L}(a, b, c)$, where $a\in\mathbb{R}$, $\mathbf{b}\in\mathbb{R}^n$, $c\in\mathbb{R}$. Given a real-valued function $u(\mathbf{x}, t)$ on $\mathbb{R}^n\times\mathbb{R}$, we form the function $F_u(\mathbf{x}, t) = \mathscr{L}(u_t, \nabla u, u)$ which is a function of $\mathbf{x}$ and t. We shall follow common practice and abuse notation in several ways. First, we shall not call the variables a, $\mathbf{b}$, c, but rather u_t, ∇u, and u. Thus, $\partial\mathscr{L}/\partial u_t$ just means the derivative of $\mathscr{L}$ on $\mathbb{R}^{n+2}$ with respect to its first variable. Moreover, when u is implicitly given, we shall write $\mathscr{L}(x, t)$ or $\mathscr{L}$ for the function denoted by $F_u(x, t)$ above. Thus, for example, a symbol like $(\partial/\partial t)(\partial\mathscr{L}/\partial u_t)$ indicates that we evaluate the function $\partial\mathscr{L}/\partial a$ by using u_t for a, etc., and then take the partial derivative with respect to t of the resulting function of $\mathbf{x}$ and t. And $\partial\mathscr{L}/\partial(\nabla u)$ denotes the n vector $\langle\partial\mathscr{L}/\partial b_1, \ldots, \partial\mathscr{L}/\partial b_n\rangle$ evaluated at u_t, ∇u, u. While these abuses are confusing, they are completely standard in the literature and quite convenient once one gets used to them.

We want to choose $\mathscr{L}$ so that the differential equation under consideration has the form of an **Euler–Lagrange** equation

$$(\mathscr{D})(u) = \frac{\partial}{\partial t}\left(\frac{\partial\mathscr{L}}{\partial u_t}\right) + \nabla\cdot\frac{\partial\mathscr{L}}{\partial(\nabla u)} - \frac{\partial\mathscr{L}}{\partial u} = 0 \tag{270j}$$

(270b) has this form if we choose

$$\mathscr{L}(u_t, \nabla u, u) = \tfrac{1}{2}u_t^2 - \tfrac{1}{2}(\nabla u)^2 - \tfrac{1}{4}u^4 \tag{270k}$$

The reason that (270j) is so useful involves the **principle of least action** or, more properly, the **principle of stationary action**: Given a bounded open region Ω in $\mathbb{R}^{n+1}$ with smooth boundary and a C^∞ function u on a neighborhood of Ω, we define the **action** by

$$A_\Omega(u) = \int_\Omega \mathscr{L}(u_t, \nabla u, u)\, d^nx\, dt$$

If v is in $C_0^\infty(\Omega)$, that is, v is C^∞ but vanishes near the boundary of Ω, then

$$\frac{d}{d\lambda}A_\Omega(u+\lambda v)\bigg|_{\lambda=0} = -\int_\Omega v(\mathscr{D})(u)\, d^3x\, dt \tag{270l}$$

so u solves (270j) if and only if, for each Ω, the action A_Ω is stationary under small changes of u *strictly inside* Ω. This gives us a way to connect the invariance properties of the equation (270j) with those of $\mathscr{L}$ itself. Consider a smooth change of coordinates

$$s = s(\mathbf{x}, t), \qquad \mathbf{y} = \mathbf{y}(\mathbf{x}, t)$$

and a smooth function V from $\mathbb{R}^{n+2}$ to $\mathbb{R}$. Let $\tilde{u}(\mathbf{x}, t)$ be defined by

$$\tilde{u}(\mathbf{x}, t) = V(u(\mathbf{y}(\mathbf{x}, t), s(\mathbf{x}, t)), \mathbf{y}(\mathbf{x}, t), s(\mathbf{x}, t))$$

When is it true that $\tilde{u}$ solves (270j) if u does? A *sufficient* condition is that $\delta\mathscr{L} = 0$ where

$$\delta\mathscr{L} \equiv [\mathscr{L}(\tilde{u})](\mathbf{x}, t) - J[\mathscr{L}(u)](\mathbf{y}(\mathbf{x}, t), s(\mathbf{x}, t)) \tag{270m}$$

where J is the determinant of the Jacobian of the transformation T: $\langle\mathbf{x}, t\rangle \to \langle\mathbf{y}, s\rangle$. The first term on the right of (270m) means compute $\mathscr{L}$ using $\tilde{u}$ in place of u. The second term means first compute $\mathscr{L}(u)$ and then make the change of variables. If $\delta\mathscr{L} = 0$, then $A_\Omega(\tilde{u}) = A_{T[\Omega]}(u)$ and thus u is stationary if and only if $\tilde{u}$ is stationary. Thus, if $\delta\mathscr{L} = 0$, then $\tilde{u}$ solves (270j) if u does. As we shall see, $\delta\mathscr{L} = 0$ is *not* necessary for the invariance of (270j) under the change of variables $u\to\tilde{u}$ (see Examples 3 and 4 below).

Noether's theorem expresses the fact that if one has a one-parameter family of transformations leaving A invariant, then one can find a conserved quantity for the corresponding Euler–Lagrange equation. The point of the above calculation was that $\delta\mathscr{L} = 0$ is sufficient for A to be invariant. In the following calculations one should think of $\langle\mathbf{x}, t\rangle$ ranging throughout $\mathbb{R}^{n+1}$

and all transformations being smooth. In fact, in applications one very often wishes to use singular transformations that are not defined on all of $\mathbb{R}^{n+1}$; the set of regions Ω is then restricted to stay away from the singular set. Although these subtleties cause some difficulties in theory, they do not in practice. For "Noether's theorem" is really just a clever way to organize the chain rule, and, at the end, one has in one's hand a candidate for a conserved quantity for the differential equation. The conservation can always be checked explicitly; the importance of Noether's theorem is that it sets up an organized scheme for providing candidates.

So, let

$$s_\varepsilon = s(\mathbf{x}, t, \varepsilon), \qquad \mathbf{y}_\varepsilon = \mathbf{y}(\mathbf{x}, t, \varepsilon)$$

be a smooth family of smooth coordinate changes and let V_ε be a smooth family of smooth maps from $\mathbb{R}^{n+2}$ to $\mathbb{R}$. Define

$$\tilde{u}_\varepsilon(\mathbf{x}, t) = V_\varepsilon(u(\mathbf{y}_\varepsilon, s_\varepsilon), \mathbf{y}_\varepsilon, s_\varepsilon)$$

Assume further that for $\varepsilon = 0$, $s_0 = t$, $\mathbf{y}_0 = \mathbf{x}$, and $V_0(u(\mathbf{y}_0, s_0), \mathbf{y}_0, s_0) = u$, so our change of variables, both dependent and independent, is the identity at $\varepsilon = 0$. Now, define

$$X_j(\mathbf{x}, t) = \left.\frac{\partial (\mathbf{y}_\varepsilon)_j}{\partial \varepsilon}\right|_{\varepsilon=0}, \qquad X_0(\mathbf{x}, t) = \left.\frac{\partial s_\varepsilon}{\partial \varepsilon}\right|_{\varepsilon=0}$$

$$\Psi(u, \mathbf{x}, t) = \left.\frac{\partial V_\varepsilon}{\partial \varepsilon}\right|_{\varepsilon=0}, \qquad S(u) = \left.\frac{\partial (\delta_\varepsilon \mathscr{L})}{\partial \varepsilon}\right|_{\varepsilon=0}$$

$$j_0 = (u_t X_0 + \nabla u \cdot \mathbf{X} + \Psi)\frac{\partial \mathscr{L}}{\partial u_t} - \mathscr{L} X_0 \tag{270n}$$

$$\mathbf{j} = (u_t X_0 + \nabla u \cdot \mathbf{X} + \Psi)\frac{\partial \mathscr{L}}{\partial (\nabla u)} - \mathscr{L}\mathbf{X} \tag{270o}$$

Then, letting $\partial_0 \equiv \partial/\partial t$:

$$\partial_0 j_0 + \nabla \cdot \mathbf{j} = S(u) \tag{270p}$$

Thus, in particular, if $\delta_\varepsilon \mathscr{L} \equiv 0$ for all ε and if $\langle j_0, \mathbf{j}\rangle$ fall off sufficiently rapidly at ∞, then $\int_{\mathbb{R}^n} j_0(x, t)\, d^n x$ is a constant. To prove (270p) we first note that

$$F \equiv \left.\frac{\partial \tilde{u}_\varepsilon}{\partial \varepsilon}\right|_{\varepsilon=0} = u_t X_0 + \nabla u \cdot \mathbf{X} + \Psi$$

So, for $\varepsilon = 0$, we can write

$$\partial_0 j_0 + \nabla \cdot \mathbf{j} = \left\{\frac{\partial \mathscr{L}}{\partial u_t}\frac{\partial F}{\partial t} + \frac{\partial \mathscr{L}}{\partial (\nabla u)} \cdot \nabla F + \left[\frac{\partial}{\partial t}\left(\frac{\partial \mathscr{L}}{\partial u_t}\right) + \nabla \cdot \left(\frac{\partial \mathscr{L}}{\partial (\nabla u)}\right)\right] F\right\}$$
$$- \frac{\partial \mathscr{L}}{\partial t} X_0 - (\nabla \mathscr{L}) \cdot \mathbf{X} - \mathscr{L}\left(\frac{\partial X_0}{\partial t} + \nabla \cdot \mathbf{X}\right) \tag{270q}$$

Using the Euler–Lagrange equation (270j), we recognize the quantity in $\{\cdot\}$ as $\partial \mathscr{L}(\tilde{u}_\varepsilon)/\partial \varepsilon|_{\varepsilon=0}$. Moreover,

$$\frac{\partial \mathscr{L}}{\partial t} X_0 + \nabla \mathscr{L} \cdot \mathbf{X} = \frac{\partial}{\partial \varepsilon}[\mathscr{L}(\mathbf{y}, s)]\bigg|_{\varepsilon=0}$$

and

$$\left.\frac{\partial J}{\partial \varepsilon}\right|_{\varepsilon=0} = \frac{\partial X_0}{\partial t} + \nabla \cdot \mathbf{X}$$

so that the right-hand side of (270q) can be recognized as $S(u)$. This proves (270p).

$j = \langle j_0, \mathbf{j}\rangle$ is called the **current** associated to the one-parameter family; and if $\partial_0 j_0 + \nabla \cdot \mathbf{j} = 0$, we say that the current is **conserved**. $S(u)$ is called the **source** for j.

Example 1 (conservation of energy and the energy-momentum tensor) Consider the equation $u_{tt} = \Delta u - F(u)$. Then, the Lagrangian is $\frac{1}{2}u_t^2 - \frac{1}{2}(\nabla u)^2 - G(u)$ where $G(y) = \int_0^y F(x)\, dx$. Clearly, the family of time translations $\langle \mathbf{x}, t\rangle \to \langle \mathbf{x}, t + \varepsilon\rangle$, $V_\varepsilon(u) = u$ leaves the equations of motion invariant and it is easy to see that $\delta \mathscr{L} = 0$ for all ε. Moreover, $\mathbf{X} = 0$, $\Psi = 0$, $X_0 = 1$. The resulting current, j_0, j_i, usually denoted by t_{00}, t_{0i}, is given by:

$$t_{00} = \tfrac{1}{2}u_t^2 + \tfrac{1}{2}(\nabla u)^2 + G(u), \qquad t_{0i} = -u_t(\nabla_i u)$$

It follows from (270j) that $\partial_0 t_{00} + \sum_{i=1}^n \partial_i t_{0i} = 0$ and we recognize $(d/dt)\int t_{00}\, dx = 0$ as conservation of energy (of course this can be computed directly by using the differential equation and integration by parts). The reason that one denotes the current with two indices is that one can just as well consider invariants under space translations $\langle \mathbf{x}, t\rangle \to \langle \mathbf{x} + \varepsilon\delta_i, t\rangle$ where $\delta_i = \langle 0, \ldots, 1, \ldots, 0\rangle$ with 1 in the ith place. The resulting current j_0, j_k is usually denoted t_{i0}, t_{ik}. One finds that

$$t_{0i} = -t_{i0} \qquad \text{and} \qquad t_{ij} = t_{ji}; \qquad 1 \le i, j \le n \tag{270r}$$

In particular, the momentum $\int u_t(\nabla_i u)\, d^n x$ is conserved. $t_{\mu\nu}$ is often called the **energy–momentum tensor**, although in fully relativistic notation, what we call $t_{\mu\nu}$ is usually called $T^{\mu}{}_{\nu}$.

Example 2 (the dilation current for (270b)) Because of the special choice of the 3 in (270b), one sees that solutions of (270b) are taken into themselves under the transformation $\langle \mathbf{x}, t\rangle \to \langle \lambda \mathbf{x}, \lambda t\rangle$; $u \to \lambda u$. For these **dilation transformations**, $\delta \mathscr{L}$ is easily seen to be zero. If we take $\lambda = e^{\varepsilon}$, then $X_0 = t$, $X_i = x_i$, $\Psi = u$. The resulting conserved quantity is

$$\int [t(\tfrac{1}{2}u_t^2 + \tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{4}u^4) + u_t \mathbf{x} \cdot \nabla u + u_t u]\, d^3x \tag{270s}$$

We have included the general form of (270p) including the source term $S(u)$ for two reasons. First the **broken invariance** occurring when $S(u) \neq 0$ can be useful; for example, if $S(u) \leq 0$ for $t \geq 0$, then (270p) implies that $\int j_0(x, t)\, d^3x \leq \int j_0(x, 0)\, d^3x$ for all $t \geq 0$ and this can be useful (see Problem 153). Secondly, if it happens that $S(u)$ is of the form $\partial_0 b_0 + \nabla \cdot \mathbf{b}$, then one finds that $\partial_0 k_0 + \nabla \cdot \mathbf{k} = 0$ for $\mathbf{k} = \mathbf{j} - \mathbf{b}$, so that k_0 is conserved. We shall first compute a broken symmetry and then turn to a class of cases where $S(u)$ is automatically of the form $\partial_0 b_0 + \nabla \cdot \mathbf{b}$.

Example 3 (broken dilation invariance for $u_{tt} = \Delta u - u|u|^{p-1}$) If $\mathscr{L} = \frac{1}{2}u_t^2 - \frac{1}{2}(\nabla u)^2 - (p+1)^{-1}|u|^{p+1}$ in three space dimensions, then under the dilation $\langle \mathbf{x}, t\rangle \to \langle \lambda \mathbf{x}, \lambda t\rangle$, $u \to \lambda u$, $\delta \mathscr{L}$ is not zero if $p \neq 3$. The part of $\mathscr{L}$ giving $u_{tt} - \Delta u$ is invariant, but

$$\delta \mathscr{L} = -(p+1)^{-1}(\lambda^{p+1} - \lambda^4)|u(\lambda \mathbf{x}, \lambda t)|^{p+1}$$

Taking $\lambda = e^{\varepsilon}$ and evaluating $\partial(\delta_\varepsilon \mathscr{L})/\partial\varepsilon$, one finds that

$$S(u) = (p+1)^{-1}(3-p)|u|^{p+1}$$

so that $S(u) \leq 0$ for $p \geq 3$. Since the dilation charge (270s) does not have obvious positivity properties, this is of limited value; but the conformal invariance which we use to prove Theorem XI.101 can be replaced by broken conformal invariance to prove the analogous result for

$$u_{tt} = \Delta u - u|u|^{p-1} \tag{270t}$$

if $3 < p < 5$ (Problem 153). Actually, this equation has a type of dilation invariance; clearly under $\langle \mathbf{x}, t\rangle \to \langle \lambda \mathbf{x}, \lambda t\rangle$, $u \to \lambda^{\alpha} u$ with $\alpha = 2(p-1)^{-1}$, solutions of (270r) go into other solutions. It is not true that $\delta \mathscr{L} = 0$ in this

case; rather $\mathscr{L}(\tilde{u}) = \lambda^{2+2\alpha}\mathscr{L}(u)(y, s)$, while $J\mathscr{L}(u)(y, s) = \lambda^{4\alpha}\mathscr{L}(u)$. This means that $A_\Omega(\tilde{u}) = \lambda^{2-2\alpha}A_{T[\Omega]}(u)$; so one can understand the invariance of the differential equation from the principle of stationary action. However $S(u) = (2-2\alpha)\mathscr{L}(u)$, so the current associated to this dilation transformation is not conserved. Moreover, S is not a divergence (Problem 154); so one cannot get a conserved current by changing from j to k. This shows that an invariance of the differential equation that is not a strict invariance of the action may not lead to a new conserved quantity.

There is one general case where $S(u)$ is automatically of the form $\partial_0 b_0 + \nabla \cdot \mathbf{b}$, namely if $\delta_\varepsilon \mathscr{L} = \partial_0 B_0^{(\varepsilon)} + \nabla \cdot \mathbf{B}^{(\varepsilon)}$; for take $b_0 = \partial B_0^{(\varepsilon)}/\partial\varepsilon$, $\mathbf{b} = \partial \mathbf{B}^{(\varepsilon)}/\partial\varepsilon$. Notice that if

$$\delta \mathscr{L} = \partial_0 B_0 + \nabla \cdot \mathbf{B} \tag{270u}$$

where $B(\mathbf{x})$ is a function only of $\tilde{u}$ and its derivatives at $\mathbf{x}$, then $A_\Omega(\tilde{u}) = A_{T(\Omega)}(u) + \int_{\partial\Omega} B_0\, d\sigma_0 + \mathbf{B} \cdot d\boldsymbol{\sigma}$, so that for $\tilde{v}$'s vanishing near $\partial\Omega$,

$$A_\Omega(\tilde{u} + \lambda\tilde{v}) - A_\Omega(\tilde{u}) = A_{T(\Omega)}(u + \lambda v) - A_{T[\Omega]}(u)$$

Thus (270p) implies that the transformation takes solutions of the Euler–Lagrange equations into other solutions. When $S(u) = \partial_0 b_0 + \nabla \cdot \mathbf{b}$, $\int (j_0 - b_0)\, d^n x$ is conserved, so that invariance of the basic differential equations may be connected with a conserved quantity different from $\int j_0\, d^n x$.

Example 4 (conformal invariance of (270b)) The inversion $z \to z^{-1}$ is analytic in the complex plane away from zero; so $u(x(x^2+y^2)^{-1}, -y(x^2+y^2)^{-1})$ is harmonic on $\mathbb{R}^2\backslash\{0\}$ if u is. Formal continuation from x to ix suggests that if $u_{tt} - u_{xx} = 0$, then $u(x(t^2-x^2)^{-1}, t(t^2-x^2)^{-1})$ also solves the wave equation away from $t^2 - x^2 = 0$, and this can be seen from straightforward calculation. In four dimensions this is no longer true; to see this consider the harmonic case first. $u(\mathbf{x}) = |\mathbf{x}|^{-2}$ is harmonic away from $\mathbf{x} = \mathbf{0}$, but $\tilde{u}(\mathbf{x}) \equiv u(\mathbf{x}|\mathbf{x}|^{-2}) = |\mathbf{x}|^2$ is not. Since the only other radially symmetric function that is harmonic is 1, one might try $\tilde{u}(\mathbf{x}) \equiv |\mathbf{x}|^{-2}u(\mathbf{x}|\mathbf{x}|^{-2})$; and, indeed, one can show by tedious calculation that $\Delta\tilde{u} = |\mathbf{x}|^{-4}(\Delta u)^{\sim}$. Similarly, for $\mathbf{x} \in \mathbb{R}^3$, $t \in \mathbb{R}$, we define the **Lorentz inversion** by

$$\mathbf{y}(t, \mathbf{x}) = \mathbf{x}(t^2 - |\mathbf{x}|^2)^{-1}, \qquad s(t, \mathbf{x}) = t(t^2 - |\mathbf{x}|^2)^{-1}$$
$$V(u, \mathbf{x}, t) = (t^2 - |\mathbf{x}|^2)^{-1}u$$

If $\tilde{u}(\mathbf{x}, t) = V(u(\mathbf{y}, s), \mathbf{y}, s)$, then $\tilde{u}$ solves $u_{tt} = \Delta u$ if and only if u does. Indeed

$$\tilde{u}_{tt} - \Delta\tilde{u} = (t^2 - |\mathbf{x}|^2)^{-2}(u_{tt} - \Delta u)^{\sim} \tag{270v}$$

Since the transformations are singular when $|\mathbf{x}| = t$, this is true only away from $|\mathbf{x}| = t$. We shall not explicitly worry about this problem below, but we note that we only show directly that $\partial_0 k_0 + \nabla \cdot \mathbf{k} = 0$ for points $\langle \mathbf{x}, t \rangle$ with $|\mathbf{x}| \neq t$ when k_0 and $\mathbf{k}$ are given by (270d) and (270i). However, k_0 and $\mathbf{k}$ are easily seen to be C^∞; so the result holds for all $\langle \mathbf{x}, t \rangle$ and therefore one obtains conservation of the conformal charge $\int k_0 \, d^3x$.

(270v) shows that $u \to \tilde{u}$ also preserves solutions of (270b). This suggests that we compute the change $\delta\mathscr{L}$ under the Lorentz inversion for the Lagrangian $\mathscr{L} = \frac{1}{2}u_t^2 - \frac{1}{2}(\nabla u)^2 - \frac{1}{4}u^4$. For this calculation, it is convenient to shift to relativistic notation: Let x_μ ($\mu = 0, 1, 2, 3$) be t, x_1, x_2, x_3, and x^μ be t, $-x_1$, $-x_2$, $-x_3$. Define $g^{\mu\nu} = g_{\mu\nu}$ to be the matrix that is zero if $\mu \neq \nu$ and that is 1 (respectively, -1) if μ and ν have the common value 0 (respectively, 1, 2, or 3). Finally, let $\partial^\mu = \partial/\partial x_\mu$. Also, we shall use the summation convention, i.e., $x^\lambda x_\lambda = t^2 - |\mathbf{x}|^2$, $\partial^\lambda \partial_\lambda = \partial_0^2 - \Delta$, etc. We begin by looking at the Jacobian matrix $T^\mu{}_\nu = \partial^\mu y_\nu$ where $y_\nu = (x^\lambda x_\lambda)^{-1} x_\nu$ is the Lorentz inversion. By direct calculation $T^\mu{}_\nu = (x^\lambda x_\lambda)^{-1} S^\mu{}_\nu$ where

$$S^\mu{}_\nu = \delta^\mu{}_\nu - 2(x^\lambda x_\lambda)^{-1} x^\mu x_\nu \tag{270w}$$

and $\delta^\mu{}_\nu$ is the unit matrix. The point is that $S^\mu{}_\nu$ is a Lorentz transformation, i.e.,

$$S^\lambda{}_\kappa \, g_{\lambda\mu} \, S^\mu{}_\nu = g_{\kappa\nu}$$

Taking determinants, we see that $|\det(S)| = 1$, so that the Jacobian $J = |\det(T)| = (x^\lambda x_\lambda)^{-4}$. Using the above invariance,

$$g_{\mu\nu} \, T^\mu{}_\kappa \, T^\nu{}_\lambda \, \partial^\kappa v \, \partial^\lambda v = (x^\lambda x_\lambda)^{-2} g_{\mu\nu} \, \partial^\mu v \, \partial^\nu v \tag{270x}$$

Now let $\tilde{u}(x) \equiv (x^\lambda x_\lambda)^{-1} u(y(x))$. Then

$$\partial^\mu \tilde{u} = (x^\lambda x_\lambda)^{-1} T^\mu{}_\nu (\partial^\nu u)(y) - 2(x^\lambda x_\lambda)^{-2} x^\mu u(y) \tag{270y}$$

If one now uses (270x) and $\mathscr{L}(u) = \frac{1}{2} g_{\mu\nu} \, \partial^\mu u \, \partial^\nu u - \frac{1}{4}u^4$, one sees that

$$\begin{aligned}(\delta\mathscr{L})(u) &= 2(x^\lambda x_\lambda)^{-3} u(y)^2 - 2(x^\lambda x_\lambda)^{-3} x_\mu u \, \partial^\mu(u(y)) \\ &= \partial_\mu B^\mu\end{aligned} \tag{270z}$$

where $B^\mu = -x^\mu (x^\lambda x_\lambda)^{-3} u(y)^2$. The terms in (270z) come from squaring (270y) and using the fact that only the square of the $\partial^\mu u$ term in $\mathscr{L}(\tilde{u})$ is cancelled by a term in $J\mathscr{L}(u)(y)$.

Lorentz inversion is not a continuous symmetry, but a single transformation. However, if we invert, then translate by $-\varepsilon$ in time, and then invert, we do get a continuous group of symmetries. Thus, we define:

$$\begin{aligned}\mathbf{y}(\mathbf{x}, t, \varepsilon) &= \mathbf{x}F, \qquad s(\mathbf{x}, t, \varepsilon) = (t - \varepsilon(t^2 - |\mathbf{x}|^2))F \\ V(\mathbf{x}, t, u, \varepsilon) &= uF \\ F(\mathbf{x}, t, \varepsilon) &= (t^2 - |\mathbf{x}|^2)[\{t - \varepsilon(t^2 - |\mathbf{x}|^2)\}^2 - |\mathbf{x}|^2]^{-1}\end{aligned}$$

This rather complicated expression is called a conformal transformation. More properly, the conformal group is the 15 parameter group of Poincaré transformations, dilations, and the conjugation of space-time translations by Lorentz inversion. Correspondingly, there are 15 conserved quantities for (270b) of which we use only two (the energy and the time component of the conformal charge) to prove Theorem XI.101, although we have also considered the momentum (three components) and dilations in this appendix.

For the above conformal transformation, we have that $\Psi = 2tu$, $X_j = 2x_j t$, $X_0 = t^2 + |\mathbf{x}|^2$ by straightforward differentiation. Thus

$$\begin{aligned}j_0 &= (|x|^2 + t^2)(\tfrac{1}{2}u_t^2 + \tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{4}u^4) + 2tu_t \mathbf{x} \cdot \nabla u + 2tu_t u \\ \mathbf{j} &= (-\nabla u)\{(|\mathbf{x}|^2 + t^2)u_t + 2t\mathbf{x} \cdot \nabla u + 2tu\} - 2t\mathbf{x}(\tfrac{1}{2}u_t^2 - \tfrac{1}{2}(\nabla u)^2 - \tfrac{1}{4}u^4)\end{aligned}$$

Given that $\delta\mathscr{L}$ is not zero for the inversion, we do not expect this for the conformal map either; but we do expect that $S(u) = \partial^\mu b_\mu$ since $\delta\mathscr{L} = \partial^\mu B_\mu$ for an inversion. As in the calculation of the inversion, $S(u)$ comes from the difference of $\frac{1}{2}(\partial^\mu \tilde{u})(\partial_\mu \tilde{u})$ and $\frac{1}{2}J(\partial^\mu u)(\partial_\mu u)$. Since

$$\tilde{u} = (1 + 2\varepsilon t)u(y) + O(\varepsilon^2)$$

we have that

$$\partial^\mu \tilde{u} = (1 + 2\varepsilon t)\partial^\mu(u(y)) + 2\varepsilon\delta^\mu{}_0 \, u + O(\varepsilon^2)$$

so the extra term is (up to $O(\varepsilon^2)$) just $\frac{1}{2}[4\varepsilon\delta^\mu{}_0 \, u(\partial^\mu u)] = \varepsilon\partial_0(u^2)$. Thus $S(u) = \partial_0(u^2)$ and therefore, if we set $\mathbf{k} = \mathbf{j}$, $k_0 = j_0 - u^2$, then $\partial_0 k_0 + \nabla \cdot \mathbf{k} = 0$. We have therefore verified that for (270b), the charge given by (270c) is conserved. More importantly, we have described how to find such conserved quantities.

XI.14 Spin wave scattering

We want to discuss a physical system that is very different from those we have discussed so far but whose scattering structure is well described by the two Hilbert space formalism we introduced in Section 3. We consider a

system of quantum mechanical spins, one at each lattice point of $\mathbb{Z}^3 \subset \mathbb{R}^3$, each interacting with its nearest neighbors. The basic states for each spin are "spin-up" and "spin-down"; but since the system is quantum mechanical, we must allow superpositions. Thus the set of states for a single spin at a fixed site $\alpha \in \mathbb{Z}^3$ is the unit sphere in a two-dimensional complex Hilbert space. If we have, at time $t = 0$, a state where one given spin is up and all the others are down, then the interactions, which we describe precisely below, are such that as the system evolves a "wave" of single spin-up states propagates through the system, that is, a time-dependent superposition of states with one spin up results with more and more weighting of sites far from the initial spin as $t \to \infty$. If we started initially with two spins up, then a superposition of states of two spins up results. If the two spins are far from one another initially, then for very small times the two spins propagate more or less as two independent single spin waves because the interactions are nearest neighbor. As they move in time, these will develop nonzero probabilities of being in a state with two neighboring spins up, which then interact and scatter. It is this process we want to describe.

This system of spins is a model (called the **Heisenberg model**) of a ferromagnet. The spins have magnetic moments and the basic interaction is magnetic. The excitations we described above are usually called **magnetic spin waves** or **magnons**. One feature to note in our system is that we have considered the spin waves in a background of all down spins, which as we shall see corresponds to a ground state of the system. One could just as well consider a system with all spins up or all spins in a fixed direction which are other possible ground states. In fact, because of an overall rotational symmetry, such theories are equivalent to the one we develop. It is only at zero absolute temperature that a system will be in a ground state; at higher temperatures one has a "superposition of excited states." There has been some deep nonrigorous work on magnons at nonzero temperatures (see the Notes).

Our discussion in this section is related to various topics which we have not yet discussed. First, we are dealing with an infinite system; and, in general, infinite systems are described most naturally in the language of C^*-algebras. This is true of the Heisenberg model at nonzero temperatures; but because one can explicitly describe the ground state of the Heisenberg magnet, one is able to avoid C^*-algebraic machinery in this case. Even here, there are other ideas that are physically and mathematically interesting, such as the phenomenon of spontaneously broken symmetry, which require C^*-algebras. We return to these ideas in later volumes. Secondly, all the scattering situations we have described thus far involve the comparison of an a priori "free dynamics" with the interacting system. In our current situation the "free dynamics" is not given by some a priori comparison system but rather by a piece of the interacting system, namely the dynamics of the one magnon states. This idea will reoccur in our study of interacting quantum field scattering in Section 16.

We first describe the model for finitely many spins. Let Λ be a finite subset of $\mathbb{Z}^3$. To each $\alpha \in \Lambda$ we associate a copy of $\mathbb{C}^2$, call it $\mathbb{C}^2_\alpha$. We refer to the vectors

$$e_1^{(\alpha)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad e_0^{(\alpha)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

respectively as the **spin up** and **spin down** states at α. The Hilbert space for finitely many spins $\mathscr{H}_\Lambda$, one at each point of Λ, is

$$\mathscr{H}_\Lambda = \bigotimes_{\alpha \in \Lambda} \mathbb{C}^2_\alpha \tag{271}$$

The set of vectors of the form $\bigotimes_{\alpha\in\Lambda} e^{(\alpha)}_{a_\alpha}$, where $\{a_\alpha\}_{\alpha \in \Lambda}$ is a sequence of zeros and ones, is a basis for $\mathscr{H}_\Lambda$; for notational convenience, we set $\psi(\{a_\alpha\}) \equiv \bigotimes_{\alpha\in\Lambda} e^{(\alpha)}_{a_\alpha}$.

In order to define the Hamiltonian H_Λ for the finite system we need some terminology. Let σ_x, σ_y, σ_z denote the Pauli matrices

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

and set $\sigma_\pm \equiv \frac{1}{2}(\sigma_x \pm i\sigma_y)$ so that

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

σ_+ flips a down spin up, and σ_- flips an up spin down. That one can think of $\frac{1}{2}\boldsymbol{\sigma}$ as the three components of a quantum angular momentum follows from the fact that they obey the commutation relations of the Lie algebra of the three-dimensional rotation group. For each $\alpha \in \Lambda$, we denote by $\sigma_x^{(\alpha)}$, $\sigma_y^{(\alpha)}$, $\sigma_z^{(\alpha)}$, $\sigma_\pm^{(\alpha)}$ the operator on $\mathscr{H}_\Lambda$ which acts (respectively) by σ_x, σ_y, σ_z, $\sigma_\pm$ on the α component of the tensor product and by the identity on the other components. Thus, in terms of the basis $\psi(\{a_\beta\})$,

$$\sigma_z^{(\alpha)}\psi(\{a_\beta\}) = (2a_\alpha - 1)\psi(\{a_\beta\})$$

$$\sigma_+^{(\alpha)}\psi(\{a_\beta\}) = \begin{cases} 0, & \text{if } a_\alpha = 1 \\ \psi(\{a_\beta + \delta_{\beta\alpha}\}), & \text{if } a_\alpha = 0 \end{cases}$$

The Hamiltonian is then defined by

$$H_\Lambda = -\tfrac{1}{2} \sum_{\substack{|\alpha-\beta|=1 \\ \alpha,\,\beta\in\Lambda}} (\sigma_z^{(\alpha)}\sigma_z^{(\beta)} + 4\sigma_+^{(\alpha)}\sigma_-^{(\beta)}) \tag{272}$$

The sum runs over all nearest-neighbor *ordered* pairs $\langle \alpha, \beta \rangle$. Because of the factor $\frac{1}{2}$, each unordered pair contributes an energy $\sigma_z^{(\alpha)}\sigma_z^{(\beta)} + 2\sigma_+^{(\alpha)}\sigma_-^{(\beta)} + 2\sigma_-^{(\alpha)}\sigma_+^{(\beta)} = \boldsymbol{\sigma}^{(\alpha)} \cdot \boldsymbol{\sigma}^{(\beta)}$ where we have set $\boldsymbol{\sigma}^{(\alpha)} = \langle \sigma_x^{(\alpha)}, \sigma_y^{(\alpha)}, \sigma_z^{(\alpha)} \rangle$. Given the connection with rotations mentioned above, the basic interaction Hamiltonian can be seen to be invariant under simultaneous rotations of all the spins. The minus sign of (272) means that states with spins parallel to each other tend to have lower energy than those antiparallel.

It can be shown (Problem 132) that if the set Λ becomes a connected set when nearest neighbors are joined, then the ground state for H_Λ is $(n+1)$-degenerate where n is the number of points in Λ. The ground state has energy $-k$ where k is the number of nearest-neighbor pairs. One of the ground state eigenvectors is $\psi_0 \equiv \bigotimes_{\alpha \in \Lambda} e_0^{(\alpha)}$. The rest of a basis of ground state eigenvectors may be obtained by applying the operator $\sum_{\alpha \in \Lambda} \sigma_+^{(\alpha)}$ some number of times.

There are two difficulties in dealing with the case $\Lambda = \mathbb{Z}^3$. First, we must decide what to take for the Hilbert space of the infinite volume system. Secondly, we must decide what to take for the Hamiltonian, especially in view of the fact that the ground state energy (that is, lowest eigenvalue) of H_Λ goes to $-\infty$ as $|\Lambda|$, the volume of Λ, goes to infinity.

One method of defining the infinite volume Hilbert space is to develop the idea of infinite tensor product and use (271); but since we shall primarily be interested in a different realization of the basic structure, we defer discussion of infinite tensor products to the Notes. We consider an infinite-dimensional Hilbert space $\mathscr{H}$ with basis $\{\psi(\{a_\beta\})\}$ where $a = \{a_\beta\}$ is a sequence of zeros and ones indexed by $\mathbb{Z}^3$ *with only finitely many* $a_\beta \neq 0$; that is, $\mathscr{H}$ consists of vectors of the form

$$\sum_a{}' \, c(a)\psi(a)$$

($\sum'$ means we allow a's only with the above italicized restriction) where $c(a) \in \mathbb{C}$ and $\sum_a' |c(a)|^2 < \infty$. The inner product on $\mathscr{H}$ is given by

$$\left(\sum{}' d(a)\psi(a), \sum{}' c(a)\psi(a)\right) = \sum{}' \overline{d(a)}c(a)$$

ψ_0 will stand for the basis vector where all the a_β are chosen equal to zero.

A complete justification for taking this Hilbert space in the infinite volume limit requires the C^*-algebraic approach, but we note that without the italicized condition the constructed Hilbert space would be inseparable while $\mathscr{H}$ is separable. Moreover, we can define $\sigma_x^{(\alpha)}$, $\sigma_y^{(\alpha)}$, $\sigma_z^{(\alpha)}$, $\sigma_\pm^{(\alpha)}$ as before and we can define a Hamiltonian H, as we shall see.

One cannot use (271) to define $H_{\mathbb{Z}^3}$ since on each $\psi(\{a_\beta\})$ the sum is divergent. However, if we replace $\sigma_z^{(\alpha)}\sigma_z^{(\beta)}$ by $\sigma_z^{(\alpha)}\sigma_z^{(\beta)} - 1$ whenever it occurs,

that is, we define

$$H_{\mathbb{Z}^3} = -\tfrac{1}{2} \sum_{\substack{|\alpha - \beta| = 1 \\ \alpha, \beta \in \mathbb{Z}^3}} (\sigma_z^{(\alpha)}\sigma_z^{(\beta)} - 1 + 4\sigma_+^{(\alpha)}\sigma_-^{(\beta)}) \tag{273}$$

then the sum converges on each $\psi(\{a_\beta\})$. Since we have just changed the ground state energy by a (infinite) constant, the physics should be the same. We now drop the $\mathbb{Z}^3$ and take the domain of H, $D(H)$, to be the dense set of finite linear combinations of the vectors $\psi(a)$. Since for each vector v in $D(H)$ all but finitely many terms of Hv are zero, H is well defined on $D(H)$. In fact:

Proposition H is essentially self-adjoint and nonnegative. ψ_0 is the unique vector with $H\psi_0 = 0$.

Proof Let $\mathscr{H}_n$ be the span of those $\psi(\{a_\beta\})$ with $\sum_\beta a_\beta = n$. Then $\mathscr{H} = \bigoplus \mathscr{H}_n$, $\mathscr{H}_n \subset D(H)$, H leaves $\mathscr{H}_n$ invariant, and H is bounded on each $\mathscr{H}_n$. It follows that H is a direct sum of bounded self-adjoint operators and so is essentially self-adjoint by an elementary argument we have used often before (see Example 2 in Section VIII.10 or Problem 1 of Chapter X). H is positive because

$$\sigma_z^{(\alpha)}\sigma_z^{(\beta)} + 2\sigma_+^{(\alpha)}\sigma_-^{(\beta)} + 2\sigma_-^{(\alpha)}\sigma_+^{(\beta)} \leq 1$$

for any α and β (Problem 131). The simplicity of the zero eigenvalue is left to the problems (Problem 133). ∎

As we have mentioned in the last proof, H leaves each subspace $\mathscr{H}_n$ invariant. Let us begin by analyzing $H \restriction \mathscr{H}_1$. For each $\alpha \in \mathbb{Z}^3$, let $\eta_\alpha = \psi(\{\delta_{\alpha\beta}\})$, that is, η_α is the vector describing the state with spin up at site α and spin down at all other sites. By definition of H and the fact that α has six nearest neighbors β_i occurring as both (α, β_i) and (β_i, α) in the sum (273),

$$H\eta_\alpha = 12\eta_\alpha - 2 \sum_{|\beta - \alpha| = 1} \eta_\beta$$

An arbitrary $\varphi \in \mathscr{H}_1$ can be expanded

$$\varphi = \sum_{\alpha \in \mathbb{Z}^3} \varphi(\alpha)\eta_\alpha$$

so $H\varphi = \sum (H\varphi)(\alpha)\eta_\alpha$ where

$$(H\varphi)(\alpha) = 2\left(6\varphi(\alpha) - \sum_{|\beta - \alpha| = 1} \varphi(\beta)\right) \tag{274}$$

To better understand $H \restriction \mathscr{H}_1$, notice that H commutes with the obvious representation of $\mathbb{Z}^3$ as translations on $\mathscr{H}$. Thus, the map of $\ell^2(\mathbb{Z}^3)$ given by $\{\varphi(\alpha)\} \mapsto \{(H\varphi)(\alpha)\}$ commutes with translations, as is obvious from (274). Thus the Fourier transform $\ell^2(\mathbb{Z}^3) \supset L^2([-\pi, \pi]^3)$ should give a spectral representation for H. Indeed, defining

$$\hat{\varphi}(k) = (2\pi)^{-3/2} \sum_{\alpha \in \mathbb{Z}^3} \varphi(\alpha) e^{-ik \cdot \alpha}$$

we find that

$$\widehat{(H\varphi)}(k) = \mu(k)\hat{\varphi}(k)$$

where

$$\mu(k) = 4(3 - \cos k_1 - \cos k_2 - \cos k_3)$$

Thus $H \restriction \mathscr{H}_1$ looks much like a lattice version of the free kinetic energy in nonrelativistic quantum mechanics since for k small, $\mu = 2|k|^2 + O(k^4)$.

We can now describe the sense in which $H \restriction \mathscr{H}_2$ is a Hamiltonian describing states that look asymptotically like two single spin waves moving freely. First we need to note that the natural two spin-wave space is not $\mathscr{H}_2$ but rather $\mathscr{H}_1 \otimes_s \mathscr{H}_1$. The reason for the symmetric tensor product is that, physically, it makes no sense to say which of the two up spins is "first." The reason for symmetry is that we have chosen the spin operators at different sites to commute, a choice based on the fact that these spins should be independent observable quantities. Had we taken the σ's to anticommute, we would have obtained a "free Fermi gas" without any scattering.

We define

$$J_2 \colon (\mathscr{H}_1 \otimes_s \mathscr{H}_1) \to \mathscr{H}_2$$

$$J_2(\eta_\alpha \otimes_s \eta_\gamma) = \begin{cases} \psi(\{\delta_{\alpha\beta} + \delta_{\gamma\beta}\}), & \alpha \neq \gamma \\ 0, & \alpha = \gamma \end{cases}$$

and use the two Hilbert space scattering theory of Section 3.

Theorem XI.102 Let $H_2 \equiv H \restriction \mathscr{H}_2$ and $H_1^{\otimes} = H_1 \otimes I + I \otimes H_1$. Then

$$\Omega_2^{\pm} = \operatorname*{s-lim}_{t \to \mp\infty} e^{+itH_2} J_2 e^{-itH_1^{\otimes}}$$

exist and are isometries of $\mathscr{H}_1 \otimes_s \mathscr{H}_1$ into $\mathscr{H}_2$.

Proof By Cook's method, the limit exists if we can prove that

$$\int_{\pm 1}^{\pm\infty} \|[H_2 J_2 - J_2 H_1^{\otimes}] e^{-itH_1^{\otimes}} \varphi\| \, dt < \infty \tag{275}$$

for a total set of φ's. Moreover, to prove that $\Omega_2^{\pm}$ are isometries, we need only show that

$$\|(J_2^* J_2 - 1) e^{-itH_1^{\otimes}} \varphi\| \to 0 \tag{276}$$

as $t \to \pm\infty$. We shall prove (275) and leave (276) to the reader (Problem 134).

Let us define $V \colon \mathscr{H}_1 \otimes_s \mathscr{H}_1 \to \mathscr{H}_1 \otimes_s \mathscr{H}_1$ by

$$V = J_2^* H_2 J_2 - H_1^{\otimes}$$

V has two important properties. First, it is bounded. Secondly, V has support in the region $|\alpha - \beta| \leq 2$ in the following sense. Identify $\mathscr{H}_1 \otimes_s \mathscr{H}_1$ with the symmetric functions in $\ell^2(\mathbb{Z}^3 \times \mathbb{Z}^3)$ by the map $\varphi \mapsto \tilde{\varphi}(\cdot, \cdot)$ where $\varphi = \sum \tilde{\varphi}(\alpha, \beta)\eta_\alpha \otimes \eta_\beta$. Define $\tilde{V}$ by $\tilde{V}\tilde{\varphi} = \widetilde{V\varphi}$. If we define an operator χ on $\ell^2(\mathbb{Z}^3 \times \mathbb{Z}^3)$ by

$$(\chi\tilde{\varphi})(\alpha, \beta) = \begin{cases} \tilde{\varphi}(\alpha, \beta), & \text{if } |\alpha - \beta| \leq 2 \\ 0, & \text{if } |\alpha - \beta| > 2 \end{cases}$$

then $\tilde{V}\chi = \tilde{V}$. This follows by noting that H_2 acts just like $H_1^{\otimes}$ as long as α and β are not nearest neighbors and do not have a neighbor in common. From now on we drop the $\tilde{}$.

Since V is so nice, we shall obtain (275) by a simple application of stationary phase ideas. Denote by $\hat{}$ the Fourier transform from $\ell^2(\mathbb{Z}^3 \times \mathbb{Z}^3)$ to $L^2([-\pi, \pi]^3 \times [-\pi, \pi]^3)$. Let φ be a vector in $\mathscr{H}_1 \otimes_s \mathscr{H}_1$ such that $\hat{\varphi} \in C_0^\infty([-\pi, \pi]^3 \times [-\pi, \pi]^3)$ and:

(i) supp $\hat{\varphi}$ does not contain any point any of whose coordinates is $\pm\pi$.
(ii) supp $\hat{\varphi} \subset \{\langle k, \ell \rangle \mid \partial\mu(k)/\partial k \neq \partial\mu(\ell)/\partial\ell\}$

Then we claim that for any $m > 0$, there are constants C_m and T so that for $t > T$,

$$|(e^{-itH_1^{\otimes}}\varphi)(\alpha, \beta)| \leq C_m(|\alpha| + |\beta| + |t| + 1)^{-m} \tag{277}$$

in the region $|\alpha - \beta| \leq 2$. For the moment, assume (277). Then, for φ as above,

$$\begin{aligned} \|J_2 V e^{-itH_1^{\otimes}}\varphi\|_{\mathscr{H}_2}^2 &\leq \|V e^{-itH_1^{\otimes}}\varphi\|_{\mathscr{H}_1 \otimes \mathscr{H}_1}^2 \\ &= \|V\chi e^{-itH_1^{\otimes}}\varphi\|_{\mathscr{H}_1 \otimes \mathscr{H}_1}^2 \\ &\leq \|V\|^2 \|\chi e^{-itH_1^{\otimes}}\varphi\|_{\mathscr{H}_1 \otimes \mathscr{H}_1}^2 \\ &= \|V\|^2 \sum_{|\alpha - \beta| \leq 2} |(e^{-itH_1^{\otimes}}\varphi)(\alpha, \beta)|^2 \\ &\leq d\|V\|^2 (1 + |t|)^{-4} \end{aligned}$$

by (277). Thus

$$\int_{\pm 1}^{\pm \infty} \|J_2 V e^{-itH_1 \otimes} \varphi\| \, dt < \infty$$

so, since $J_2 J_2^* = I$, we conclude that (275) holds. Since the set of such φ's are dense, the wave operators exist.

The proof of (277) is a simple exercise in the stationary phase machinery of the first appendix to Section 3; in fact only the elementary Theorem XI.14 is necessary. For, let $\omega = |\alpha| + |\beta| + |t|$ and

$$f_{\alpha,\beta,t}(k, \ell) = (\alpha \cdot k + \beta \cdot \ell - t\mu(k) - t\mu(\ell))(|\alpha| + |\beta| + |t|)^{-1}$$

Then

$$(e^{-itH_1 \otimes} \varphi)(\alpha, \beta) = \text{const} \int e^{i\omega f_{\alpha,\beta,t}(k,\ell)} \hat{\varphi}(k, \ell) \, dk \, d\ell$$

obeys (277) by Theorem XI.14 and the conditions (i) and (ii). ∎

There is little problem in extending the above ideas to n-spin waves; we use notation allowing all n at once. Let $\mathscr{F}_1$ be the Fock space built on $\mathscr{H}_1$. One defines

$$J: \mathscr{F}_1 \to \mathscr{H}$$

by mapping $\otimes_s^n \mathscr{H}_1$ onto $\mathscr{H}_n$ via

$$J(\eta_{\alpha_1} \otimes \cdots \otimes \eta_{\alpha_n}) = \begin{cases} \psi(\{\delta_{\alpha_1 \beta} + \cdots + \delta_{\alpha_n \beta}\}), & \text{all } \alpha\text{'s unequal} \\ 0, & \text{otherwise} \end{cases}$$

Then, by mimicking the above proof, one easily sees that:

Theorem XI.103

$$\Omega^{\pm} = \text{s-lim}_{t \to \mp \infty} e^{itH} J e^{-it d\Gamma(H_1)}$$

exist and are isometries.

If $\varphi \in \otimes_s^n \mathscr{H}_1$, then $\Omega^{\pm} \varphi$ are states that asymptotically look like n free spin waves. We have just defined scattering states corresponding to a system with n spins flipped decaying into n pieces. Motivated by the N-body Schrödinger case, one can ask if there are not other channels corresponding to bound clusters of some of the flipped spins. There are, but these "bound states" have an additional complexity not present in the Schrödinger case. In the latter case the center of mass motion factors out of the full Hamiltonian, so that "bound states" are eigenvectors of a fixed operator. The key fact there is that if $\mu_S(\mathbf{k}) = k^2$, and $\sum_1^N \mathbf{k}_i = 0$, then

$$\sum_{i=1}^N \mu_S(\mathbf{a} + \mathbf{k}_i) = f(\mathbf{a}) + \sum_{i=1}^N \mu_S(\mathbf{k}_i)$$

so, for arbitrary $\mathbf{k}_i$, $\sum_{i=1}^N \mu_S(\mathbf{k}_i)$ is the sum of one function of $\mathbf{K} = \mathbf{k}_1 + \cdots + \mathbf{k}_N$ alone and one function of $\mathbf{k}_1 - \mathbf{k}_2, \ldots, \mathbf{k}_{N-1} - \mathbf{k}_N$, alone. This fails for the function $\mu(\mathbf{k}) = 3 - \cos k_1 - \cos k_2 - \cos k_3$. "Removing the center of mass motion" in a spin wave system corresponds then to realizing $H_n \equiv H \restriction \mathscr{H}_n$ as

$$(H_n \varphi)(K, k_1, \ldots, k_{n-1}) = (H_n(K) \varphi_K)(k_1, \ldots, k_{n-1})$$

where $K = k_1 + \cdots + k_n$ and $H_n(K)$ is a K-dependent operator. H_n is realized as a "fibered operator" in the sense to be discussed in Section XIII.16, or in another parlance as a "direct integral." K is the total momentum which commutes with H_n. A "bound state" is then an eigenvalue of $H_n(K)$ for some fixed K which typically varies continuously as K varies. When such "bound states" are present (and they are in the system discussed above; see the Notes), one can construct additional wave operators for the associated channels as in the Schrödinger case.

One can prove asymptotic completeness of scattering on $\mathscr{H}_2$ (Problem 135).

XI.15 Quantum field scattering I: The external field

You might think that this is a question that could be asked seriously only by a field theorist driven mad by spending too many years in too few dimensions. — *S. Coleman*

In this section and the next we discuss scattering in quantum field theory. In Section 16 we show that in a field theory that satisfies the Wightman axioms and certain additional hypotheses, there is a natural way to construct a scattering operator. This general theory, called the Haag-Ruelle theory, is both elegant and important since it shows conceptually how the Wightman fields are related to the scattering of individual particles. Unfortunately, the construction of dynamics for nontrivial field theories and the verification of the Wightman axioms is very difficult and so far has been accomplished only for models in one and two space dimensions. In this

section we discuss what should be a much simpler problem, scattering in an external field. This problem should be simpler because the interacting field satisfies a *linear* wave equation, for example,

$$\varphi_{tt}(x, t) - \Delta\varphi(x, t) + m^2\varphi(x, t) = V(x, t)\varphi(x, t) \tag{278}$$

where $V(x, t)$ is the external potential.

One important phenomenon associated with the quantized version of (278) is the phenomenon of pair creation. If one starts initially with a no particle state, the expectation value of the field will be nonzero; and, as a result, because of the linearity of (278) the right-hand side will act as a source term and be nonzero. That is, there will be a nonzero probability that pairs of particles will be produced.

The phenomenon of pair creation has two striking consequences in the mathematical structure of the theory. First, the "free" dynamics at $t = -\infty$ will be different from the "free" dynamics at $t = +\infty$. Secondly, the theory is complicated in that there must be scattering amplitudes which describe the scattering of n incoming particles into m outgoing particles. It turns out that all these amplitudes can be described in terms of a certain fundamental solution of the *classical* field equation.

Before beginning the discussion of (278), we would like to describe some of the reasons external field problems are interesting. First, because external field problems are "explicitly solvable," they have often been used as approximations to and as a guide for understanding fully interacting cases. One place where the approximation has been used is in nuclear physics where the nucleon field is treated as an external field for the mesons. This is thought to be reasonable because the nucleons are so much heavier than the mesons. A place where external field problems have been used as a guide is the treatment of infrared problems in quantum electrodynamics. Secondly, certain Yukawa fields can be expressed as integrals over external fields after the fermions "have been integrated out." The external fields in this problem are not smooth and reflect the ultraviolet difficulties. Thirdly, there are a large number of invariant wave equations to choose from in the case of higher spin as well as a variety of couplings, and one would like to know which of the associated free fields are stable under coupling to an external field. If the free fields are unstable under external field coupling (that is, if the coupled theory has various pathologies), then one presumes that coupling to a fully quantized interacting field would be even worse. What is becoming apparent is that there are *no* equations of spin $\frac{3}{2}$ or greater that possess completely nonpathological external field couplings. This is not necessarily a disaster since particles of spin $\frac{3}{2}$ can arise in theories where the fields have spin $\frac{1}{2}$ (see the Notes to Section IX.8). More serious is the problem that the

gravitational field in Einstein's equations has spin 2. Two ways out of this dilemma have been suggested: One is that the gravitational equations have very special nonlinearities which may not be well modeled by external fields. A more spectacular speculation is that the graviton might be a bound state of two photons and the "gravitational field"—a derived object!

In this section we shall consider only the spin zero case with the coupling (278). We assume that $V(x, t)$ is a C^∞ real-valued function of x and t with compact support. Our aim is to construct a quantum field satisfying (278) and all the Wightman axioms except Poincaré invariance (we cannot expect Poincaré invariance to hold since V is not Poincaré invariant) and then to develop a scattering theory. The great advantage of having a linear equation of motion for the field is that we can use the analogous classical wave equation to generate the quantum field dynamics. Thus we begin by studying the existence and scattering theory for the classical wave equation

$$\begin{aligned} w_{tt} - \Delta w + m^2 w &= V(x, t)w \\ w(x, 0) &= w_1(x) \\ w_t(x, 0) &= w_2(x) \end{aligned} \tag{279}$$

As in Section 10, we set $B = \sqrt{-\Delta + m^2}$ and rewrite (279) as a first-order system

$$\frac{d}{dt}\begin{pmatrix} w \\ w_t \end{pmatrix} = \begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix}\begin{pmatrix} w \\ w_t \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ V & 0 \end{pmatrix}\begin{pmatrix} w \\ w_t \end{pmatrix}$$

To make the later transition to the field theory problem easy, it is convenient to diagonalize the free part of the dynamics in the following way. Let

$$T = \frac{1}{\sqrt{2}}\begin{pmatrix} B^{1/2} & iB^{-1/2} \\ B^{1/2} & -iB^{-1/2} \end{pmatrix}$$

We set $\mathcal{H} = L^2(\mathbb{R}^3)$, take $\mathcal{H} \oplus \mathcal{H}$ as our Hilbert space, and define operators h_0 and $v(t)$ by

$$-ih_0 \equiv T\begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix}T^{-1} = i\begin{pmatrix} -B & 0 \\ 0 & B \end{pmatrix}$$

$$-iv(t) \equiv T\begin{pmatrix} 0 & 0 \\ V & 0 \end{pmatrix}T^{-1} = \frac{i}{2}B^{-1/2}V(x, t)B^{-1/2}\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}$$

If we define $\eta(t) = \langle \alpha(t), \beta(t) \rangle = T\langle w(t), w_t(t) \rangle$, then (279) becomes

$$\begin{aligned} \eta'(t) &= -ih_0\eta(t) - iv(t)\eta(t) \\ \eta(0) &= \langle \alpha_0(x), \beta_0(x) \rangle \equiv T\langle w(0), w_t(0) \rangle \end{aligned} \tag{280}$$

for the $(\mathcal{h} \oplus \mathcal{h})$-valued function $\eta(t)$. h_0 is self-adjoint on $D(h_0) = D(B) \oplus D(B)$ and $v(t)$ is a continuous function from $\mathbb{R}$ into the bounded operators on $\mathcal{h} \oplus \mathcal{h}$ satisfying

$$\|v(t)\|_{\mathscr{L}(\mathcal{h}\oplus\mathcal{h})} \leq 2m^{-1} \sup_{x,t} |V(x, t)| \equiv M < \infty$$

Thus, for each t,

$$ih(t) \equiv i(h_0 + v(t))$$

is the generator of an exponentially bounded semigroup on $\mathcal{h} \oplus \mathcal{h}$, and all the $ih(t)$ have $D(h_0)$ as common domain by Theorem X.50. Further, since we are assuming that $V(x, t)$ is continuously differentiable, it is easy to check (Problem 137) that the operators $ih(t) + M + 1$ satisfy hypotheses (a)–(c) of Theorem X.70. Thus, Theorem X.70 implies that there exists a continuous family $u(t, s)$ of bounded operators on $\mathcal{h} \oplus \mathcal{h}$ so that $u(t, s)\eta_0$ is differentiable for $\eta_0 \in D(h_0)$ and

$$\begin{aligned} \frac{d}{dt} u(t, s)\eta_0 &= -ih(t)u(t, s)\eta_0 \\ u(s, s)\eta_0 &= \eta_0 \end{aligned} \tag{281}$$

Further, because of the bound on $\|v(t)\|$, $u(t, s)$ satisfies $\|u(t, s)\eta_0\| \leq e^{M|t-s|}\|\eta_0\|$. Notice that since $-ih(t)$ also generates an exponentially bounded semigroup, $u(t, s)$ is defined for all t and s and satisfies $u(t_1, t_2)u(t_2, t_3) = u(t_1, t_3)$. Since the propagation backward in time satisfies the same estimate as above, we have

$$e^{-M|t-s|}\|\eta_0\| \leq \|u(t, s)\eta_0\| \leq e^{M|t-s|}\|\eta_0\| \tag{282}$$

for all t and s. We remark that since the perturbations are bounded, we could have used the Dyson series in the interaction picture to define the dynamics (see the discussion after Theorem X.69) instead of the more subtle Theorem X.70.

The family of operators $T^{-1}u(t, s)T$ has two other important properties. First, the propagation is causal. That is, if $w_0 = \langle w(x, s), w_t(x, s)\rangle$ has support in Σ, then $w(t) = T^{-1}u(t, s)Tw_0$ has support in $\{x \,|\, |x - y| \leq |t - s| \text{ for some } y \in \Sigma\}$. The idea of the proof is exactly as in Theorem X.77 except that the nonlinear term $-|u|^2u$ is replaced by $V(x, t)w$. Secondly, let λ denote the operator

$$\lambda = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

on $\mathcal{h} \oplus \mathcal{h}$. Then,

$$u(t, s)^*\lambda u(t, s) = \lambda = u(t, s)\lambda u(t, s)^* \tag{283a}$$

for all t and s.

Before proving (283a), we note that, in terms of the original variables, it is equivalent to the statement that

$$q \equiv \int_{\mathbb{R}^3} [\overline{w(x, t)}w_t(x, t) - w(x, t)\overline{w_t(x, t)}]\, d^3x \tag{283b}$$

is independent of time for solutions w of (279). After we quantize, (283a) will express the conservation of "charge." To prove (283a) we note that by the boundedness of $u(t, s)$ and polarization, we need just show that

$$(u(t, s)\eta_0, \lambda u(t, s)\eta_0) = (\eta_0, \lambda\eta_0) = (u(t, s)^*\eta_0, \lambda u(t, s)^*\eta_0)$$

for η_0 in a dense set. It thus suffices to show that (283b) is time independent for solutions of (279) with initial data in $C_0^\infty(\mathbb{R}^3)$. The solution is then in $C_0^\infty(\mathbb{R}^3)$ for all times. Moreover, (283b) is just the Wronskian of the two solutions w and $\bar{w}$ of (279) and so is independent of time because the necessary integration by parts is permissible since $w(\cdot, t) \in C_0^\infty(\mathbb{R}^3)$. In terms of Noether's theorem, described in the appendix to Section 13, the conservation of q is an expression of the invariance $w \mapsto e^{i\theta}w$ (Problem 152).

We summarize:

Theorem XI.104 Let $V(x, t)$ be a continuously differentiable function of compact support in $\mathbb{R}^4$. Let $\mathcal{h} \oplus \mathcal{h}$, h_0 and $v(t)$ be as defined above. Then there exists a strongly continuous two-parameter family $u(t, s)$ of bounded operators on $\mathcal{h} \oplus \mathcal{h}$ such that:

(a) $u(t_3, t_2)u(t_2, t_1) = u(t_3, t_1)$; $u(t, t) = I$.
(b) If $\eta_0 \in D(h_0)$, then (281) holds and $\eta(t) = u(t, 0)\eta(0)$ satisfies (280).
(c) If supp $w(0) \in \Sigma$, then supp $T^{-1}u(t, 0)Tw(0) \subset \{x \,|\, |x - y| \leq |t - s| \text{ for some } y \in \Sigma\}$.
(d) (283a) holds.
(e) Let $w_1 \in D(B^2)$ and $w_2 \in D(B)$ and set $\langle \alpha, \beta\rangle = T\langle w_1, w_2\rangle$. Define $\langle \alpha(t), \beta(t)\rangle \equiv u(t, 0)\langle \alpha, \beta\rangle$. Then $w(t) = 2^{-1/2}\{B^{-1/2}\alpha(t) + B^{-1/2}\beta(t)\}$ is twice differentiable as an $L^2(\mathbb{R}^3)$-valued function and satisfies (279) with initial data $w(0) = w_1$, $w_t(0) = w_2$.

We have already proven (a)–(d). (e) holds because (279) and (280) are equivalent; one need only check the domain details (Problem 138).

We now introduce a classical interaction picture which will later be useful in the field theory situation. Let

$$\tilde{u}(t, s) = e^{ith_0}u(t, s)e^{-ish_0}$$

Then, for $\eta_0 \in D(h_0)$,

$$\frac{d}{dt}\tilde{u}(t, s)\eta_0 = e^{ith_0}(-iv(t))u(t, s)e^{-ish_0}\eta_0$$

$$= e^{+ith_0}(-iv(t))e^{-ith_0}(e^{+ith_0}u(t, s)e^{-ish_0})\eta_0$$

so $\tilde{u}(t, s)\eta_0$ satisfies

$$\frac{d}{dt}\tilde{u}(t, s)\eta_0 = -i\tilde{v}(t)\tilde{u}(t, s)\eta_0$$

$$\tilde{u}(s, s)\eta_0 = \eta_0$$

where

$$\tilde{v}(t) = e^{+ith_0}v(t)e^{-ith_0}$$

Notice that by (282) and $u(s, t)u(t, s) = u(s, s) = I$, both $u(t, s)$ and $\tilde{u}(t, s)$ are bounded operators with bounded inverses.

We turn next to the classical scattering theory for (280) which is very easy because of our strong assumptions on $V(x, t)$. Let $u_0(t)$ denote e^{-ith_0} and let t_0 be large enough so that $v(x, t) = 0$ for $|t| \geq t_0$. Let $\eta_- \in \mathcal{h} \oplus \mathcal{h}$ be given and define $W_+\eta_-$ to be that vector in $\mathcal{h} \oplus \mathcal{h}$ so that

$$\|u_0(t)\eta_- - u(t, 0)(W_+\eta_-)\|_{\mathcal{h}\oplus\mathcal{h}} \to 0 \qquad \text{as} \quad t \to -\infty \tag{284}$$

By part (a) of Theorem XI.104,

$$\eta(x, t) \equiv u(t, -t_0)u_0(-t_0)\eta_-(x) = u(t, 0)u(0, -t_0)u_0(-t_0)\eta_-(x)$$

Moreover, for $t < -t_0$, $u(t, -t_0) = u_0(t + t_0)$ since $v(t) = 0$ for $t < -t_0$. Thus, for $t < -t_0$,

$$\eta(x, t) = u_0(t + t_0)u_0(-t_0)\eta_-(x) = u_0(t)\eta_-(x)$$

so if we set

$$W_+\eta_- = u(0, -t_0)u_0(-t_0)\eta_-$$

then (284) holds since the norm is zero for $t < -t_0$. Similarly,

$$W_-\eta_+ = u(0, t_0)u_0(t_0)\eta_+$$

Since both u_0 and u are surjective, Ran $W_+ = \mathcal{h} \oplus \mathcal{h} =$ Ran W_-, so we have asymptotic completeness and

$$\begin{aligned} S_{\text{cl}} = W_-^{-1}W_+ &= [u(0, t_0)u_0(t_0)]^{-1}[u(0, -t_0)u_0(-t_0)] \\ &= u_0(-t_0)u(t_0, 0)u(0, -t_0)u_0(-t_0) \\ &= u_0(-t_0)u(t_0, -t_0)u_0(-t_0) \\ &= \tilde{u}(t_0, -t_0) \end{aligned}$$

Thus the classical scattering operator is just the interaction picture propagator from $-t_0$ to t_0.

We turn now to the field theory problem and begin by introducing the charged free scalar field of mass m. Let $\mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3))$ be the boson Fock space over $L^2(\mathbb{R}^3)$ and let $a^\dagger(\cdot)$ and $a(\cdot)$ be the creation and annihilation operators on $\mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3))$ occurring in (X.74), (X.75), and (X.76). As, in Section X.7, we denote by F_0 the finite particle vectors and set

$$D_{\mathscr{S}} = \{\psi \in F_0 \,|\, \psi^{(n)} \in \mathscr{S}(\mathbb{R}^{3n}) \quad \text{for all } n \geq 1\}$$

Let $\mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3))$ be another copy of the same Fock space on which we denote the corresponding annihilation and creation operators by $b(\cdot)$ and $b^\dagger(\cdot)$. If $\mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3))$ is the Hilbert space for some boson and $\mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3))$ is the Hilbert space of the corresponding antiparticles, then the Hilbert space of the combined system is

$$\mathscr{H} \equiv \mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3)) \otimes \mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3)) = \mathscr{F}_s(\mathcal{h} \oplus \mathcal{h})$$

For each $f \in \mathcal{h}$, $a(f)$, $a^\dagger(f)$, $b(f)$, $b^\dagger(f)$ can be naturally identified with operators $a(f) \otimes I$, $a^\dagger(f) \otimes I$, $I \otimes b(f)$, $I \otimes b^\dagger(f)$ on $\mathscr{H}$ which we shall denote simply by $a(f)$, $a^\dagger(f)$, $b(f)$, and $b^\dagger(f)$ also. As described in Section X.7, one defines operator-valued distributions $a(p)$, $a^\dagger(p)$, $b(p)$, $b^\dagger(p)$. In terms of these annihilation and creation operators on $\mathscr{H}$ we define the **free Hamiltonian**

$$H_0 \equiv \int_{\mathbb{R}^3} \mu(p)a^\dagger(p)a(p)\, d^3p + \int_{\mathbb{R}^3} \mu(p)b^\dagger(p)b(p)\, d^3p$$

where $\mu(p) = \sqrt{p^2 + m^2}$, the **number operators**

$$N_+ \equiv \int_{\mathbb{R}^3} a^\dagger(p)a(p)\, d^3p$$

$$N_- \equiv \int_{\mathbb{R}^3} b^\dagger(p)b(p)\, d^3p$$

and the **charge operator**,

$$Q \equiv N_+ - N_-$$

Using Nelson's analytic vector theorem, it is easy to check that H_0, N_+, N_-, and Q are essentially self-adjoint on $D_{\mathscr{S}} \otimes D_{\mathscr{S}}$ which we shall denote simply by $D_{\mathscr{S}}$ from now on. We define the **charged free scalar Boson field** as the operator-valued distribution (note that the subscript zero refers to "free" and not to "time zero"):

$$\varphi_0(f, t) = \frac{1}{\sqrt{2}}\{a(e^{-iBt}B^{-1/2}f) + b^\dagger(e^{iBt}B^{-1/2}f)\}$$

for $f \in \mathscr{h}$. Formally, $\varphi_0(x, t)$ is just given by

$$\varphi_0(x, t) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} [e^{-i(\mu(p)t - p\cdot x)}a(p) + e^{i(\mu(p)t - p\cdot x)}b^\dagger(p)] \frac{d^3p}{\sqrt{2\mu(p)}}$$

We also define the **time-zero fields** by

$$\varphi_0(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} (e^{ip\cdot x}a(p) + e^{-ip\cdot x}b^\dagger(p)) \frac{d^3p}{\sqrt{2\mu(p)}}$$

$$\pi_0(x) \equiv \varphi_0(x)^* = \frac{i}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} (e^{-ip\cdot x}a^\dagger(p) - e^{ip\cdot x}b(p)) \sqrt{\frac{\mu(p)}{2}}\, d^3p$$

$\varphi_0(x, t)$ is given in terms of the time zero field $\varphi_0(x)$ by the formula

$$\varphi_0(f, t) = e^{iH_0t}\varphi_0(f)e^{-iH_0t}$$

The creation and annihilation operators satisfy the commutation relations

$$[a(f), a^\dagger(g)] = (f, g)_{L^2}$$
$$[b(f), b^\dagger(g)] = (f, g)_{L^2}$$
$$[a^*(f), b^*(g)] = 0$$

for real-valued $f, g \in L^2(\mathbb{R}^3)$ where # denotes either a dagger or not.

If $\mathscr{U}^{(1)}$ and $\mathscr{U}^{(2)}$ are the actions of the Lorentz group on $\mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3))$ and $\mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3))$, we take $\mathscr{U} = \mathscr{U}^{(1)} \otimes \mathscr{U}^{(2)}$ to be the representation here. Finally, notice that we have a vacuum $\psi_0 = \psi_0^{(1)} \otimes \psi_0^{(2)}$ defined in terms of the vacua $\psi_0^{(i)}$ in $\mathscr{F}_s^{(i)}(L^2(\mathbb{R}^3))$. The quadruple $\langle \mathscr{H}, \mathscr{U}, \varphi_0(x, t), F_0 \rangle$ satisfies the obvious extension of the Gårding–Wightman axioms to non-Hermitian fields. This fact and the others claimed above may be verified just as in the case of the Hermitian scalar field discussed in Section X.7 (Problem 139).

Our problem is to solve the operator-valued Cauchy problem, that is, to find an operator-valued distribution $\varphi(x, t)$ that satisfies

$$\frac{d^2}{dt^2}\varphi(x, t) - \Delta\varphi(x, t) + m^2\varphi(x, t) = V(x, t)\varphi(x, t)$$
$$\varphi(x, 0) = \varphi_0(x) \tag{285}$$
$$\frac{d}{dt}\varphi(x, 0) = \pi_0(x)^*$$

We proceed analogously to the classical case and first solve

$$\frac{d}{dt}\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix} = i\begin{pmatrix} -B & 0 \\ 0 & B\end{pmatrix}\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix} + \frac{i}{2}B^{-1/2}VB^{-1/2}\begin{pmatrix} 1 & 1 \\ -1 & -1\end{pmatrix}\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix}$$
$$= -i(h_0 + v(t))\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix} \tag{286}$$
$$a(x, 0) = a(x), \qquad b^\dagger(x, 0) = b^\dagger(x)$$

where $a(x)$ is the inverse Fourier transform of $a(p)$ and where the equation is supposed to hold in the (operator-valued) distributional sense. Since the equation is *linear*, we can solve it using the classical solution. If

$$u(t, 0) = \begin{pmatrix} u_{11}(t) & u_{12}(t) \\ u_{21}(t) & u_{22}(t)\end{pmatrix}$$

with $u_{ij}(t)$: $\mathscr{h} \to \mathscr{h}$, then, at least formally,

$$\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix} = \begin{pmatrix} u_{11}(t) & u_{12}(t) \\ u_{21}(t) & u_{22}(t)\end{pmatrix}\begin{pmatrix} a(x) \\ b^\dagger(x)\end{pmatrix}$$

Thus, for $f \in \mathscr{h}$, we define the operator-valued distributions $a(\cdot, t)$ and $b^\dagger(\cdot, t)$ by

$$a(f, t) = a(u_{11}^{\mathrm{T}}(t)f) + b^\dagger(u_{12}^{\mathrm{T}}(t)f)$$
$$b^\dagger(f, t) = a(u_{21}^{\mathrm{T}}(t)f) + b^\dagger(u_{22}^{\mathrm{T}}(t)f)$$

where $u_{ij}^{\mathrm{T}}(t)$, the transpose of $u_{ij}(t)$ on $\mathscr{h}$, is related to $u_{ij}(t)^*$ by $u_{ij}^{\mathrm{T}}(t) = Cu_{ij}(t)^*C$. We caution the reader that throughout the transposes are on

$\mathcal{h} = L^2(\mathbb{R}^3)$ and are not taken with respect to the two-by-two matrix structure. Finally, we define $\varphi(\cdot, t)$ and $\pi(\cdot, t)$ by

$$\begin{aligned}\varphi(f, t) &= \frac{1}{\sqrt{2}}\{a(B^{-1/2}f, t) + b^\dagger(B^{-1/2}f, t)\} \\ &= \frac{1}{\sqrt{2}}\{a((u_{11}^{\mathrm{T}}(t) + u_{21}^{\mathrm{T}}(t))B^{-1/2}f) \\ &\quad + b^\dagger((u_{12}^{\mathrm{T}}(t) + u_{22}^{\mathrm{T}}(t))B^{-1/2}f)\} \qquad (287a)\end{aligned}$$

$$\begin{aligned}\pi(\bar{f}, t)^* &= \frac{i}{\sqrt{2}}\{-a(B^{1/2}f, t) + b^\dagger(B^{1/2}f, t)\} \\ &= \frac{i}{\sqrt{2}}\{a((-u_{11}^{\mathrm{T}}(t) + u_{21}^{\mathrm{T}}(t))B^{1/2}f) \\ &\quad + b^\dagger((-u_{12}^{\mathrm{T}}(t) + u_{22}^{\mathrm{T}}(t))B^{1/2}f)\} \qquad (287b)\end{aligned}$$

$\pi(\cdot, t)$ is only defined for $f \in D(B^{1/2})$. Because of (281), we have the following relations:

$$\begin{aligned}u_{11}'(t) + u_{21}'(t) &= -iB(u_{11}(t) - u_{21}(t)) \\ u_{12}'(t) + u_{22}'(t) &= iB(-u_{12}(t) + u_{22}(t)) \\ u_{11}''(t) + u_{21}''(t) &= (-B^2 + B^{1/2}VB^{-1/2})(u_{11}(t) + u_{21}(t)) \\ u_{12}''(t) + u_{22}''(t) &= (-B^2 + B^{1/2}VB^{-1/2})(u_{12}(t) + u_{22}(t))\end{aligned}$$

Thus for $f \in D(B)$ real-valued,

$$\begin{aligned}\frac{d}{dt}\varphi(f, t) &= \frac{i}{\sqrt{2}}\{a([-B(u_{11}(t) - u_{21}(t)]^{\mathrm{T}}B^{-1/2}f) \\ &\quad + b^\dagger([B(-u_{12}(t) + u_{22}(t))]^{\mathrm{T}}B^{-1/2}f)\} \\ &= \frac{i}{\sqrt{2}}\{-a((u_{11}^{\mathrm{T}}(t) - u_{21}^{\mathrm{T}}(t))B^{1/2}f) \\ &\quad + b^\dagger((-u_{12}^{\mathrm{T}}(t) + u_{22}^{\mathrm{T}}(t))B^{1/2}f)\} \\ &= \pi(f, t)^*\end{aligned}$$

and, similarly, for $f \in D(B^2)$,

$$\frac{d^2}{dt^2}\varphi(f, t) = \varphi(-B^2 f, t) + \varphi(Vf, t)$$

which shows that $\varphi(\cdot, t)$ satisfies (285) in the sense of distributions.

In terms of the operators $a(f, t)$, $b^\dagger(f, t)$, we define in the natural way

$$\begin{aligned}a^\dagger(f, t) &= a(Cf, t)^* \\ b(f, t) &= b^\dagger(Cf, t)^*\end{aligned}$$

Then at time t these operators satisfy the canonical commutation relations:

$$\begin{aligned}[a(f, t), a^\dagger(g, t)] &= (Cf, g) \\ [b(f, t), b^\dagger(g, t)] &= (Cf, g) \\ [a^*(f, t), b^*(g, t)] &= 0\end{aligned}$$

To see why this is true, note that

$$\begin{aligned}a(f, t) &= a(u_{11}^{\mathrm{T}}f) + b^\dagger(u_{12}^{\mathrm{T}}f) \\ a^\dagger(g, t) &= a(u_{11}^{\mathrm{T}}Cg)^* + b^\dagger(u_{12}^{\mathrm{T}}Cg)^* \\ &= a^\dagger(Cu_{11}^{\mathrm{T}}Cg) + b(Cu_{12}^{\mathrm{T}}Cg) \\ &= a^\dagger(u_{11}^*g) + b(u_{12}^*g)\end{aligned}$$

Thus

$$\begin{aligned}[a(f, t), a^\dagger(g, t)] &= [a(u_{11}^{\mathrm{T}}f), a^\dagger(u_{11}^*g)] + [b^\dagger(u_{12}^{\mathrm{T}}f), b(u_{12}^*g)] \\ &= (Cu_{11}^{\mathrm{T}}f, u_{11}^*g) - (Cu_{12}^*g, u_{12}^{\mathrm{T}}f) \\ &= (u_{11}^*Cf, u_{11}^*g) - (u_{12}^*Cf, u_{12}^*g) \\ &= (Cf, (u_{11}u_{11}^* - u_{12}u_{12}^*)g) \\ &= (Cf, g)\end{aligned}$$

since $u_{11}u_{11}^* - u_{12}u_{12}^* = I$ by (283a). The other commutators are computed similarly. It follows that

$$[\varphi(f, t), \pi(g, t)] = i(Cf, g)$$

Finally, we check that the field $\varphi(x, t)$ is causal, that is, that

$$[\varphi(f, t), \varphi(g, t')] = 0 \qquad (288a)$$

$$[\varphi(f, t), \varphi(g, t')^*] = 0 \qquad (288b)$$

if the sets $\{\langle x, t\rangle \mid x \in \operatorname{supp} f\}$ and $\{\langle x, t'\rangle \mid x \in \operatorname{supp} g\}$ are spacelike separated. Since $a(f)$ commutes with $a(g)$ for all f and g and similarly for $b(\cdot)$, (288a) holds automatically. We shall prove (288b) in the case where

$t' = 0$. The general case is proven similarly using the relation $u(t_1, t_2)u(t_2, t_3) = u(t_1, t_3)$ (Problem 140).

$$\begin{aligned}[\varphi(f, t), \varphi(g)^*] &= \tfrac{1}{2}[a((u_{11} + u_{21})^{\mathrm{T}}B^{-1/2}f), a^\dagger(CB^{-1/2}g)] \\ &\quad + \tfrac{1}{2}[b^\dagger((u_{12} + u_{22})^{\mathrm{T}}B^{-1/2}f, b(CB^{-1/2}g)] \\ &= \tfrac{1}{2}(C(u_{11} + u_{21})^{\mathrm{T}}B^{-1/2}f, CB^{-1/2}g) \\ &\quad - \tfrac{1}{2}(B^{-1/2}g, (u_{21} + u_{22})^{\mathrm{T}}B^{-1/2}f) \\ &= \tfrac{1}{2}((u_{11} + u_{21})^*CB^{-1/2}f, CB^{-1/2}g) \\ &\quad - \tfrac{1}{2}((u_{21} + u_{22})^*CB^{-1/2}f, CB^{-1/2}g) \\ &= \tfrac{1}{2}(Cf, B^{-1/2}\{(u_{11} + u_{21}) - (u_{12} + u_{22})\}B^{-1/2}Cg)\end{aligned}$$

Now let

$$d(t) = \begin{pmatrix} d_{11}(t) & d_{12}(t) \\ d_{21}(t) & d_{22}(t) \end{pmatrix} \equiv T^{-1}u(t, 0)T$$

Then $d_{12}(t) = B^{-1/2}\{(u_{11} + u_{21}) - (u_{12} + u_{22})\}B^{-1/2}$. Since the solution of the classical equation is causal, Theorem XI.104c, we conclude that $(Cf, d_{12}(t)Cg)$ is zero for $t < T$ if the supports of f and g are separated by a distance T.

We summarize:

Theorem XI.105 Let $\varphi(f, t)$ and $\pi(f, t)$ be given by (287). Then $\varphi(\cdot, t)$ and $\pi(\cdot, t)$ are operator-valued distributions and

(a) $\varphi(\cdot, t)$ satisfies (285) where $\varphi_0(x)$ and $\pi_0(x)$ are the free time zero fields.

(b) $\dfrac{d}{dt}\varphi(\cdot, t) = \pi(\cdot, t)^*$.

(c) At each time t, $\varphi(\cdot, t)$ and $\pi(\cdot, t)$ satisfy the canonical commutation relations $[\varphi(f, t), \pi(g, t)] = i(Cf, g)$.

(d) Microscopic causality holds.

We turn now to the problem of scattering in the external field $V(x, t)$. Let $\varphi_{\mathrm{in}}(x, t)$ denote the free charged scalar field of mass m with associated annihilation and creation operators a_{in} and $a_{\mathrm{in}}^\dagger$. As before $V(x, t)$ is a real-valued function that is zero for $|t| \geq t_0$. We would like to solve the initial value problem

$$\frac{d^2}{dt^2}\varphi(x, t) - \Delta\varphi(x, t) + m^2\varphi(x, t) = V(x, t)\varphi(x, t) \tag{289}$$

$$\varphi(x, -t_0) = \varphi_{\mathrm{in}}(x, -t_0)$$

$$\dot{\varphi}^*(x, -t_0) = \pi_{\mathrm{in}}(x, -t_0)$$

If we define

$$a_{\mathrm{in}}(f, t) \equiv e^{iHot}a_{\mathrm{in}}(f)e^{-iHot} = a_{\mathrm{in}}(e^{-iBt}f)$$

$$b_{\mathrm{in}}^\dagger(f, t) \equiv e^{iHot}b_{\mathrm{in}}^\dagger(f)e^{-iHot} = b_{\mathrm{in}}^\dagger(e^{iBt}f)$$

Then $\varphi_{\mathrm{in}}(x, -t_0)$ and $\pi_{\mathrm{in}}(x, -t_0)$ are given in terms of $a_{\mathrm{in}}(x)$ and $b_{\mathrm{in}}^\dagger(x)$ by the formulas

$$\begin{aligned}\varphi_{\mathrm{in}}(f, -t_0) &= \frac{1}{\sqrt{2}}\{a_{\mathrm{in}}(B^{-1/2}f, -t_0) + b_{\mathrm{in}}^\dagger(B^{-1/2}f, -t_0)\} \\ &= \frac{1}{\sqrt{2}}\{a_{\mathrm{in}}(e^{iBto}B^{-1/2}f) + b_{\mathrm{in}}^\dagger(e^{-iBto}B^{-1/2}f)\}\end{aligned}$$

and

$$\pi_{\mathrm{in}}(f, -t_0)^* = \frac{i}{\sqrt{2}}\{-a_{\mathrm{in}}(e^{iBto}B^{1/2}f) + b_{\mathrm{in}}^\dagger(e^{-iBto}B^{1/2}f)\}$$

We can solve the initial value problem (289) analogously to the way we solved the initial value problem at $t = 0$. Set $u(t) = u(t, -t_0)$ and define

$$a(x, t) \equiv u_{11}(t)a_{\mathrm{in}}(x, -t_0) + u_{12}(t)b_{\mathrm{in}}^\dagger(x, -t_0)$$

$$b^\dagger(x, t) \equiv u_{21}(t)a_{\mathrm{in}}(x, -t_0) + u_{22}(t)b_{\mathrm{in}}^\dagger(x, -t_0)$$

and

$$\begin{aligned}\varphi(f, t) &\equiv \frac{1}{\sqrt{2}}\{a(B^{-1/2}f, t) + b^\dagger(B^{-1/2}f, t)\} \\ &= \frac{1}{\sqrt{2}}\{a_{\mathrm{in}}((u_{11}^{\mathrm{T}} + u_{21}^{\mathrm{T}})B^{-1/2}f, -t_0) \\ &\quad + b_{\mathrm{in}}^\dagger((u_{12}^{\mathrm{T}} + u_{22}^{\mathrm{T}})B^{-1/2}f, -t_0)\} \\ &= \frac{1}{\sqrt{2}}\{a_{\mathrm{in}}(e^{iBto}(u_{11}^{\mathrm{T}} + u_{21}^{\mathrm{T}})B^{-1/2}f) \\ &\quad + b_{\mathrm{in}}^\dagger(e^{-iBto}(u_{12}^{\mathrm{T}} + u_{22}^{\mathrm{T}})B^{-1/2}f)\} \\ \pi(f, t)^* &\equiv \frac{i}{\sqrt{2}}\{a_{\mathrm{in}}(e^{iBto}(-u_{11}^{\mathrm{T}} + u_{21}^{\mathrm{T}})B^{1/2}f) \\ &\quad + b_{\mathrm{in}}^\dagger(e^{-iBto}(-u_{12}^{\mathrm{T}} + u_{22}^{\mathrm{T}})B^{1/2}f)\}\end{aligned}$$

Then, as above $d\varphi(f, t)/dt = \pi(f, t)$ and $\varphi(x, t)$ satisfies (289) in the sense of distributions. In fact, $\varphi(x, t) = \varphi_{in}(x, t)$ for all $t \leq -t_0$.

Since $\varphi(x, t)$ satisfies (289) and $V(x, t) = 0$ for $t \geq t_0$, we have

$$\frac{d^2}{dt^2}\varphi(x, t) - \Delta\varphi(x, t) + m^2\varphi(x, t) = 0, \qquad t \geq t_0$$

That is, $\varphi(x, t)$ satisfies the free field equation for $t \geq t_0$. This suggests that we define

$$a_{out}(x, t_0) = u_{11}(t_0, -t_0)a_{in}(x, -t_0) + u_{12}(t_0, -t_0)b_{in}^\dagger(x, -t_0)$$
$$b_{out}^\dagger(x, t_0) = u_{22}(t_0, -t_0)a_{in}(x, -t_0) + u_{22}(t_0, -t_0)b_{in}^\dagger(x, -t_0)$$

and

$$\varphi_{out}(f, t) = \frac{1}{\sqrt{2}}\{a_{out}(e^{-i(t-t_0)B}B^{-1/2}f, t_0) + b_{out}^\dagger(e^{i(t-t_0)B}B^{-1/2}f, t_0)\}$$
$$\pi_{out}(f, t)^* = \frac{i}{\sqrt{2}}\{-a_{out}(e^{-i(t-t_0)B}B^{1/2}f, t_0) + b_{out}^\dagger(e^{i(t-t_0)B}B^{1/2}f, t_0)\}$$

For $f \in \mathscr{S}$, $a_{out}(f, t)$, $b_{out}^\dagger(f, t)$, $\varphi_{out}(f, t)$, and $\pi_{out}(f, t)$ and all their products are well-defined operators on $D_{\mathscr{S}}$. Further, $d\varphi_{out}(f, t)/dt = \pi_{out}(f, t)$ and $\varphi_{out}(x, t)$ is a "free field" in the sense that it satisfies the free Klein–Gordon equation for all t. Notice also that $\varphi(x, t) = \varphi_{out}(x, t)$ for all $t \geq t_0$. We shall see later, though it is not obvious a priori, that there is a vacuum ψ_{out} for the out fields, that

$$H_{out} = \int_{\mathbb{R}^3} \mu(p)a_{out}^\dagger(p, t_0)a_{out}(p, t_0)\, d^3p + \int_{\mathbb{R}^3} \mu(p)b_{out}^\dagger(p, t_0)b_{out}(p, t_0)\, d^3p \tag{290}$$

makes sense as a self-adjoint operator on $\mathscr{H}$ and that

$$\varphi_{out}(x, t) = e^{iH_{out}(t-t_0)}\varphi_{out}(x, t_0)e^{-iH_{out}(t-t_0)}$$
$$\pi_{out}(x, t) = e^{iH_{out}(t-t_0)}\pi_{out}(x, t_0)e^{-iH_{out}(t, -t_0)}$$

Since a_{out} has some $b_{in}^\dagger$ in it, H_{out} will not annihilate ψ_{in}, so $H_{out} \neq H_{in} \equiv H_0$. Thus, the asymptotic free dynamics near $t = +\infty$ is not the same as the asymptotic free dynamics near $t = -\infty$. The dynamical situation is described by Fig. XI.15. In accordance with the general ideas of this chapter we should define a scattering transformation $\mathfrak{S}$ as a map from

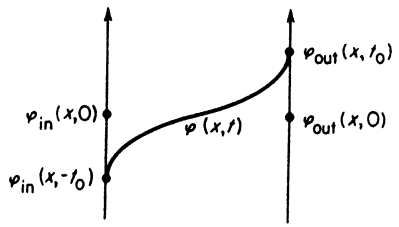


FIGURE XI.15

operators to operators given by

$$\mathfrak{S}\colon \varphi_{in}(x, 0) \to \varphi_{out}(x, 0)$$
$$\mathfrak{S}\colon \pi_{in}(x, 0) \to \pi_{out}(x, 0)$$

We shall see that $\mathfrak{S}$ is unitarily implementable, that is, that there exists a unitary operator S on $\mathscr{H}$ such that

$$\varphi_{out}(f, 0) = S^{-1}\varphi_{in}(f, 0)S$$
$$\pi_{out}(f, 0) = S^{-1}\pi_{in}(f, 0)S$$

We shall call S the **scattering operator** and $\mathfrak{S}$ the **Heisenberg picture scattering operator** since $\mathfrak{S}$ represents the scattering transformation in the Heisenberg picture of quantum mechanics. Notice that S can only be determined up to a phase by these conditions. The convention on S corresponds to using the Jauch S-matrix as opposed to the EBFM S-matrix which we have used thus far in this volume. This choice is universal in field theory and we will use it again in the next section. We have the following explicit action of $\mathfrak{S}$:

$$\begin{aligned}\mathfrak{S}(a_{in}(f)) &= a_{out}(f, 0)\\ &= \frac{1}{\sqrt{2}}\{\varphi_{out}(f, 0) + i\pi(f, 0)^*\}\\ &= a_{out}(e^{it_0B}f, t_0)\\ &= a_{in}(u_{11}^\dagger(t_0, -t_0)e^{it_0B}f, -t_0)\\ &\quad + b_{in}^\dagger(u_{12}^\dagger(t_0, -t_0)e^{it_0B}f, -t_0)\\ &= a_{in}(e^{it_0B}u_{11}^\dagger(t_0, -t_0)e^{it_0B}f)\\ &\quad + b_{in}^\dagger(e^{-it_0B}u_{12}^\dagger(t_0, -t_0)e^{it_0B}f)\\ &= a_{in}(\tilde{u}_{11}^\dagger(t_0, -t_0)f) + b_{in}^\dagger(\tilde{u}_{12}^\dagger(t_0, -t_0)f)\end{aligned}$$

and similarly

$$\begin{aligned}\mathfrak{S}(b_{in}^\dagger(f)) &= b_{out}^\dagger(f, 0)\\ &= a_{in}(\tilde{u}_{21}^\dagger(t_0, -t_0)f) + b_{in}^\dagger(\tilde{u}_{22}^\dagger(t_0, -t_0)f)\end{aligned}$$

Thus the transformation from time zero annihilation and creation operators of the in field to the time zero annihilation and creation operators of the out field is given by

$$\begin{pmatrix} a_{\text{out}}(x,0) \\ b^\dagger_{\text{out}}(x,0) \end{pmatrix} = S_{\text{cl}} \begin{pmatrix} a_{\text{in}}(x) \\ b^\dagger_{\text{in}}(x) \end{pmatrix}$$

where

$$S_{\text{cl}} = \tilde{u}(t_0, -t_0) = e^{it_0 h_0} u(t_0, -t_0) e^{it_0 h_0}$$

is the classical scattering operator.

We seek to construct a unitary S so that

$$\begin{aligned} S^{-1} a^*_{\text{in}}(f) S &= a^*_{\text{out}}(f) \\ S^{-1} b^*_{\text{in}}(f) S &= b^*_{\text{out}}(f) \end{aligned} \tag{291}$$

where $a^\dagger_{\text{out}}, b_{\text{out}}$ are given in terms of $a_{\text{out}}, b^\dagger_{\text{out}}$ by the usual formulas involving the conjugation C. Since h_0 commutes with λ and (283) holds, $\tilde{u}(t_0, -t_0)$ satisfies

$$\tilde{u}(t_0, -t_0)^* \lambda \tilde{u}(t_0, -t_0) = \lambda = \tilde{u}(t_0, -t_0) \lambda \tilde{u}(t_0, -t_0)^* \tag{292}$$

Thus, the same proof as in Theorem XI.105 shows that $a_{\text{out}}, b_{\text{out}}$ satisfy the canonical commutation relations

$$\begin{aligned} [a_{\text{out}}(f,0), a^\dagger_{\text{out}}(g,0)] &= (Cf, g) \\ [b_{\text{out}}(f,0), b^\dagger_{\text{out}}(g,0)] &= (Cf, g) \end{aligned}$$

and that all other commutators vanish.

The following theorem reduces the question of unitary implementability to a property of the classical propagation.

Theorem XI.106 Suppose that $\tilde{u}_{11}(t_0, -t_0)^{-1} \tilde{u}_{12}(t_0, -t_0)$ is a Hilbert-Schmidt operator on $L^2(\mathbb{R}^3)$. Then there is a unitary operator S on $\mathscr{H} = \mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3)) \otimes \mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3))$ so that (291) holds.

Proof Since $\tilde{u}$ satisfies (292), we have that

$$\tilde{u}^*_{11} \tilde{u}_{11} = 1 + \tilde{u}^*_{12} \tilde{u}_{12}, \qquad \tilde{u}_{11} \tilde{u}^*_{11} = 1 + \tilde{u}_{12} \tilde{u}^*_{12} \tag{293}$$

so $\tilde{u}^*_{11} \tilde{u}_{11} \geq 1$ and $\tilde{u}_{11} \tilde{u}^*_{11} \geq 1$, from which it follows that Ran $\tilde{u}_{11} = L^2(\mathbb{R}^3)$ and that $\tilde{u}_{11}^{-1}$ exists and is bounded. Thus, $\tilde{u}_{11}(t_0, -t_0)^{-1} \tilde{u}_{12}(t_0, -t_0)$ makes sense.

To prove the theorem we construct a vector ψ_{out} in $\mathscr{H}$ which is a vacuum for the out fields. Once this is done, it will be easy to write down S^{-1} explicitly.

According to Theorems VI.17 and VI.22e and the hypothesis, there exist orthonormal sets $\{f_i\}, \{g_i\}$ in $L^2(\mathbb{R}^3)$ so that $L = \tilde{u}_{11}^{-1} \tilde{u}_{12}$ may be written

$$Lh = \sum_{i=1}^{N_0} \lambda_i (g_i, h) f_i$$

where the λ_i are the eigenvalues of $|L|$ and $\sum \lambda_i^2 < \infty$. N_0 may be finite or infinite; we will consider the case $N_0 = \infty$ since that is where most of the difficulties occur. From (293) it follows that

$$1 = LL^* + (\tilde{u}_{11}^{-1})(\tilde{u}_{11}^{-1})^* \tag{294}$$

and since $LL^* h = \sum \lambda_i^2 (f_i, h) f_i$, it follows that $\lambda_i \leq 1$ since $(\tilde{u}_{11}^{-1})(\tilde{u}_{11}^{-1})^* \geq 0$. Furthermore, if $\lambda_{i_0} = 1$ for some i_0, (294) implies that $(\tilde{u}_{11}^{-1})^* f_i = 0$, which is impossible since Ran $\tilde{u}_{11}^{-1} = L^2(\mathbb{R}^3)$. Thus, $\lambda_i < 1$ for all i.

Now, denote the vacuum in $\mathscr{H}$ by ψ_{in} and let F_{in} be the set of finite linear combination of vectors of the form $\psi_1 \otimes \psi_2$ where $\psi_i \in F_0 \subset \mathscr{F}_s(L^2(\mathbb{R}^3))$. In terms of the orthonormal sets $\{f_i\}, \{g_i\}$, we define

$$a_i = a_{\text{in}}(Cf_i), \qquad b_i = b_{\text{in}}(g_i)$$

The out vacuum is given formally by

$$\psi_{\text{out}} = d \left(\prod_{i=1}^{\infty} e^{-\lambda_i a_i^* b_i^*} \right) \psi_{\text{in}}$$

where the constant d is chosen so that $\|\psi_{\text{out}}\| = 1$. To make sense out of this expression let us begin by looking at $e^{-\lambda_1 a_1^* b_1^*} \psi_{\text{in}}$ which we define by the power series

$$e^{-\lambda_1 a_1^* b_1^*} \psi_{\text{in}} = \sum_{n=0}^{\infty} \frac{(-\lambda_1 a_1^* b_1^*)^n}{n!} \psi_{\text{in}}$$

For each n, ψ_{in} is in the domain of $(a_1^* b_1^*)^n$ and

$$\begin{aligned} (a_1^* b_1^*)^n \psi_{\text{in}} &= \left[\sqrt{n!}\, S_n \left(\overset{n}{\otimes} f_1 \right) \right] \otimes \left[\sqrt{n!}\, S_n \left(\overset{n}{\otimes} \bar{g}_1 \right) \right] \\ &= n! \left(\overset{n}{\otimes} f_1 \right) \otimes \left(\overset{n}{\otimes} \bar{g}_1 \right) \end{aligned}$$

For different n, the vectors $(a_1^* b_1^*)^n \psi_{\text{in}}$ are orthogonal, so

$$\begin{aligned} \| e^{-\lambda_1 a_1^* b_1^*} \psi_{\text{in}} \|^2 &= \sum_{n=0}^{\infty} \frac{\lambda_1^{2n}}{(n!)^2} \| (a_1^* b_1^*)^n \psi_{\text{in}} \|^2 \\ &= \sum_{n=0}^{\infty} \lambda_1^{2n} = \frac{1}{1 - \lambda_1^2} \end{aligned}$$

Thus $e^{-\lambda_1 a_1^* b_1^*}\psi_{\text{in}}$ makes sense since $\lambda_1 < 1$. Similarly, using the fact that $(f_1, f_2) = 0 = (g_1, g_2)$, we have

$$(a_2^* b_2^*)^{n-s}(a_1^* b_1^*)^s \psi_{\text{in}} = \left[\sqrt{n!}\, S_n\left(\overset{n-s}{\otimes} f_2 \otimes \overset{s}{\otimes} f_1\right)\right] \otimes \left[\sqrt{n!}\, S_n\left(\overset{n-s}{\otimes} \bar{g}_2 \otimes \overset{s}{\otimes} \bar{g}_1\right)\right]$$

so

$$\|(a_2^* b_2^*)^{n-s}(a_1^* b_1^*)^s \psi_{\text{in}}\|^2 = (n!)^2\left[\frac{(n-s)!s!}{n!}\right]^2 = [(n-s)!s!]^2$$

Thus

$$\begin{aligned}
&\|e^{-\lambda_2 a_2^* b_2^*} e^{-\lambda_1 a_1^* b_1^*}\psi_{\text{in}}\|^2 \\
&= \left\|\sum_{n=0}^{\infty} \frac{1}{n!}(-\lambda_1 a_1^* b_1^* - \lambda_2 a_2^* b_2^*)^n \psi_{\text{in}}\right\|^2 \\
&= \sum_{n=0}^{\infty}\left(\frac{1}{n!}\right)^2 \sum_{s=0}^{n}\left(\frac{n!}{(n-s)!s!}\right)^2 \lambda_1^{2s}\lambda_2^{2(n-s)}\|(a_2^* b_2^*)^{n-s}(a_1^* b_1^*)^s\psi_{\text{in}}\|^2 \\
&= \sum_{n=0}^{\infty}\sum_{s=0}^{n}\lambda_1^{2s}\lambda_2^{2(n-s)} \\
&= \frac{1}{1-\lambda_1^2}\frac{1}{1-\lambda_2^2}
\end{aligned}$$

Continuing in this way, we show that

$$\chi_N = \left(\prod_{i=1}^{N} e^{-\lambda_i a_i^* b_i^*}\right)\psi_{\text{in}}$$

exists and that

$$\|\chi_N\|^2 = \prod_{i=1}^{N}\left(\frac{1}{1-\lambda_i^2}\right)$$

Furthermore, using the orthogonality of the $\{f_i\}$ among themselves and the $\{g_i\}$ among themselves, it follows similarly to the above calculation (Problem 141a) that

$$\|\chi_N - \chi_M\|^2 = \prod_{i=1}^{N}\left(\frac{1}{1-\lambda_i^2}\right) - \prod_{i=1}^{M}\left(\frac{1}{1-\lambda_i^2}\right) \tag{295}$$

Because of the Hilbert–Schmidt assumption, $\sum \lambda_i^2 < \infty$, so the infinite product $\prod_{i=1}^{\infty}(1-\lambda_i^2)^{-1}$ converges. Thus, χ_N is Cauchy as $N \to \infty$ and we define the limit, suitably normalized, as ψ_{out}.

To prove that ψ_{out} is annihilated by $a_{\text{out}}(f)$ recall that

$$a_{\text{out}}(f) = a_{\text{in}}(\tilde{u}_{11}^{\mathrm{T}} f) + b_{\text{in}}^{\dagger}(\tilde{u}_{12}^{\mathrm{T}} f)$$

Since $\operatorname{Ran}(\tilde{u}_{11}^{\mathrm{T}})^{-1} = L^2(\mathbb{R}^3)$, we may suppose that f is of the form $f = (\tilde{u}_{11}^{\mathrm{T}})^{-1}h$. Choose $h = Cf_i$. Then

$$\begin{aligned}
a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1}Cf_i) &= a_{\text{in}}(Cf_i) + b_{\text{in}}^{\dagger}(\tilde{u}_{12}^{\mathrm{T}}(\tilde{u}_{11}^{\mathrm{T}})^{-1}Cf_i) \\
&= a_{\text{in}}(Cf_i) + b_{\text{in}}^{\dagger}(C((\tilde{u}_{11})^{-1}\tilde{u}_{12})^* f_i) \\
&= a_{\text{in}}(Cf_i) + b_{\text{in}}^{\dagger}(C\lambda_i g_i) \\
&= a_i + \lambda_i b_i^*
\end{aligned}$$

By the orthogonality of the $\{f_i\}$ and $\{g_i\}$, the a_i^* and b_i^* all commute for different i, so

$$\begin{aligned}
(a_i + \lambda_i b_i^*)\chi_N &= \left(\prod_{j\neq i}^{N} e^{-\lambda_j a_j^* b_j^*}\right)(a_i + \lambda_i b_i^*)e^{-\lambda_i a_i^* b_i^*}\psi_{\text{in}} \\
&= 0
\end{aligned}$$

since $(a_i + \lambda_i b_i^*)e^{-\lambda_i a_i^* b_i^*}\psi_{\text{in}} = 0$ on account of the canonical commutation relations satisfied by a_i and a_i^* (Problem 141b). Letting $N \to \infty$ we see that ψ_{out} is in the domain of $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1}Cf_i)$ and that $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1}Cf_i)\psi_{\text{out}} = 0$. Suppose that $k \in \{f_i\}^{\perp}$. Then $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1}Ck) = a_{\text{in}}(Ck)$ and since $a_{\text{in}}(Ck)$ commutes with a_i^* and b_i^* for all i, we conclude that $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1}Ck)\psi_{\text{out}} = 0$ also. Expanding an arbitrary $h \in L^2(\mathbb{R}^3)$ in terms of $\{f_i\}$ and a basis for $\{f_i\}^{\perp}$, one easily shows from this that ψ_{out} is in the domain of $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1}h)$ and that $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1}h)\psi_{\text{out}} = 0$. The proof that b_{out} annihilates ψ_{out} is similar and uses $\tilde{u}_{21}^*(\tilde{u}_{22}^*)^{-1} = \tilde{u}_{11}^{-1}\tilde{u}_{12}$ which follows from the fact that $\tilde{u}$ satisfies (292).

Define

$$h_i = (\tilde{u}_{11}^{-1}) * f_i/\sqrt{1-\lambda_i^2}, \qquad k_i = (\tilde{u}_{22}^{-1}) * g_i/\sqrt{1-\lambda_i^2}$$

and

$$\tilde{a}_i \equiv a_{\text{out}}(Ch_i), \qquad \tilde{b}_i \equiv b_{\text{out}}(k_i)$$

Then, calculating as above,

$$\tilde{a}_i = a_{\text{in}}(\tilde{u}_{11}^{\mathrm{T}} Ch_i) + b_{\text{in}}^{\dagger}(\tilde{u}_{12}^{\mathrm{T}} Ch_i) = \frac{a_i + \lambda_i b_i^*}{\sqrt{1-\lambda_i^2}}$$

and

$$\tilde{b}_i = \frac{b_i + \lambda_i a_i^*}{\sqrt{1-\lambda_i^2}}$$

It follows easily from (294) that $\{h_i\}$ is an orthonormal set. To see that $\{k_i\}$ is an orthonormal set, one first uses (283a) to prove that

$$\begin{aligned}\sum_{i=1}^{\infty} \lambda_i^2 (g_i, \cdot) g_i &= LL^* \\ &= \tilde{u}_{22}^{-1}\tilde{u}_{21}\tilde{u}_{21}^*(\tilde{u}_{22}^{-1})^* \\ &= I - \tilde{u}_{22}^{-1}(\tilde{u}_{22}^{-1})^*\end{aligned}$$

from which the orthonormality follows easily. We now extend $\{h_i\}$ to an orthonormal basis for $L^2(\mathbb{R}^3)$ which we denote by $\{\eta_i\}$ and extend $\{Ck_i\}$ to an orthonormal basis which we denote by $\{\gamma_i\}$. For vectors of the form $\prod a_{\text{in}}^\dagger(\eta_i)\prod b_{\text{in}}^\dagger(\gamma_j)\psi_{\text{in}}$, we define S^{-1} by

$$S^{-1}: \psi_{\text{in}} \to \psi_{\text{out}}$$

$$S^{-1}\prod a_{\text{in}}^\dagger(\eta_i)\prod b_{\text{in}}^\dagger(\gamma_j)\psi_{\text{in}} \to \prod a_{\text{out}}^\dagger(\eta_i)\prod b_{\text{out}}^\dagger(\gamma_j)\psi_{\text{out}}$$

where the products are taken over some finite collections of i's and j's. First, notice that the right-hand side makes sense because ψ_{out} is in the domain of $\prod a_{\text{out}}^\dagger(\eta_i)\prod b_{\text{out}}^\dagger(\gamma_j)$. If $\eta_i = (\tilde{u}_{11}^{-1})^* f_i/\sqrt{1-\lambda_i^2}$, then

$$a_{\text{out}}^\dagger(\eta_i) = (a_i^* + \lambda_i b_i)/\sqrt{1-\lambda_i^2}.$$

On the other hand, if η_i is one of the other basis elements, then $\eta_i = (\tilde{u}_{11}^{-1})^* f$ where $f \in \{f_i\}^\perp$ and $\|f\| = 1$. This is because (294) implies that $(\tilde{u}_{11}^{-1})^*$ is an isometry from $\{f_i\}^\perp$ to $\{(\tilde{u}_{11}^{-1})^*[\{f_i\}]\}^\perp$. So, in this case $a_{\text{out}}^\dagger(\eta_i) = a_{\text{in}}(Cf)^*$ where $f \perp \{f_i\}$. Similar statements hold for the $a_{\text{out}}^\dagger(\gamma_i)$ based on properties of $(\tilde{u}_{22}^{-1})^*$. Thus each term in $\prod a_{\text{out}}^\dagger(\eta_i)\prod b_{\text{out}}^\dagger(\gamma_j)$ is a product of a finite number of powers of a_i^*, b_i^*, $a_{\text{in}}(Cf)$, $b_{\text{in}}(g)$. When such products are applied to χ_N the asserted limit (ψ_{out}) still exists since a_i^*, b_i^* do not affect χ_N for $N > i$ and $a_{\text{in}}(Cf)$, $b_{\text{in}}(g)$ commute with $e^{-\lambda_i a_i^* b_i^*}$ for all i and, when taken inside, do not affect the estimates because $f \perp \{f_i\}$, $g \perp \{g_i\}$. This same orthogonality and the definitions of $\tilde{a}_i$, $\tilde{b}_i$ ensure that $a_{\text{out}}^\dagger(\eta_i)$, $a_{\text{out}}(C\eta_i)$, $b_{\text{out}}^\dagger(\gamma_i)$, $b_{\text{out}}(C\gamma_i)$ satisfy the canonical commutation relations, from which it follows that S^{-1} is norm preserving and orthogonality preserving on the orthonormal basis $\{\prod a_{\text{in}}^\dagger(\eta_i)\prod b_{\text{in}}^\dagger(\gamma_i)\psi_{\text{in}}\}$ for $\mathscr{H}$. Thus S^{-1} extends uniquely to an isometry of $\mathscr{H}$ into $\mathscr{H}$, and it is easy to check that (291) holds. The reader is asked to fill in the details of the above argument in Problem 141c.

In order to show that S^{-1} is unitary we need just show that S^{-1} has a dense range and to do that it is sufficient to show that every vector of the form $\prod a_{\text{in}}^\dagger(\eta_i)\prod b_{\text{in}}^\dagger(\gamma_i)\psi_{\text{in}}$ can be approximated by finite linear combinations of vectors of the form $\prod a_{\text{out}}^\dagger(\eta_i)\prod b_{\text{out}}^\dagger(\gamma_i)\psi_{\text{out}}$. To see that this is so, define $\psi'_{\text{in}} = d'\prod_{i=1}^{\infty} e^{\lambda_i a_i^* b_i^*}\psi_{\text{out}}$. The same proofs as in the construction of ψ_{out} show that the right-hand side converges and that $a_{\text{in}}(C\eta_i)\psi'_{\text{in}} = 0 = b_{\text{in}}(C\gamma_j)\psi'_{\text{in}}$ for all i and j. Thus, adjusting the constant d', we have $\psi'_{\text{in}} = \psi_{\text{in}}$, and

$$\prod a_{\text{in}}^\dagger(\eta_i)\prod b_{\text{in}}^\dagger(\gamma_i)\psi_{\text{in}} = \prod a_{\text{in}}^\dagger(\eta_i)\prod b_{\text{in}}^\dagger(\gamma_i)\, d'\prod_{n=1}^{\infty} e^{\lambda_n a_n^* b_n^*}\psi_{\text{out}}.$$

Since $a_{\text{in}}^\dagger(\eta_i)$ and $b_{\text{in}}^\dagger(\gamma_i)$ can be expressed in terms of $\tilde{a}_i^*$, $\tilde{b}_i^*$, or directly in terms of $a_{\text{out}}^\dagger$, $b_{\text{out}}^\dagger$, and we can make the infinite product finite and terminate the remaining exponentials after finitely many terms, the left-hand side can be approximated by finite linear combinations of terms of the form $\prod a_{\text{out}}^\dagger(\eta_i)\prod b_{\text{out}}^\dagger(\gamma_j)\psi_{\text{out}}$ as required. ∎

Before proving that $\tilde{u}_{12}(t_0, -t_0)$ is Hilbert–Schmidt, we make several remarks about the proof just completed. First, the argument can be turned around to show that if the map $a_{\text{in}} \to a_{\text{out}}$, $b_{\text{in}} \to b_{\text{out}}$ is unitarily implementable, then $\tilde{u}_{11}^{-1}\tilde{u}_{12}$ is Hilbert–Schmidt. Secondly, the proof depended only on the Hilbert–Schmidt hypothesis and (292) and so the same proof together with the proposition below shows that for each t, there is a unitary operator $U(t, -t_0)$ so that

$$\begin{aligned}\varphi(x, t) &= U(t, -t_0)\varphi_{\text{in}}(x, -t_0)U(t, -t_0)^{-1} \\ \pi(x, t) &= U(t, -t_0)\pi_{\text{in}}(x, -t_0)U(t, -t_0)^{-1}\end{aligned}$$

that is, the dynamics given by Theorem XI.105 is unitarily implementable. Finally, if we set $H_{\text{out}} = S^{-1}H_{\text{in}}S$, then H_{out} is given by

$$H_{\text{out}} = \int_{\mathbb{R}^3} \mu(p) a_{\text{out}}^\dagger(p, 0) a_{\text{out}}(p, 0)\, dp + \int_{\mathbb{R}^3} \mu(p) b_{\text{out}}^\dagger(p, 0) b_{\text{out}}(p, 0)\, dp$$

H_{out} is also given by (290), and the free dynamics of the out fields is given by $e^{itH_{\text{out}}}$. All of these facts are trivial once one has S since they are just the translations of facts about the (free) in field.

Proposition Suppose that $V(x, t)$ is C^∞ with compact support in $\mathbb{R}^4$. Then the operators $u_{12}(t, -t_0)$ and $\tilde{u}_{12}(t, -t_0)$ described above are Hilbert–Schmidt on $L^2(\mathbb{R}^3)$.

Proof Since $u_{12}(t, s) = e^{-itB}\tilde{u}_{12}(t, s)e^{-isB}$, it suffices to prove that $\tilde{u}_{12}(t, -t_0)$ is Hilbert-Schmidt. Since $t \to \tilde{v}(t)$ is a strongly continuous map of $\mathbb{R}$ into the bounded operators on $L^2(\mathbb{R}^3)$, $\tilde{u}(t, -t_0)$ is given by the Dyson series (Theorem X.69):

$$\tilde{u}(t, -t_0)f = f + \sum_{n=1}^{\infty} (-i)^n \int_{-t_0}^{t} \int_{-t_0}^{t_1} \cdots \int_{-t_0}^{t_{n-1}} \tilde{v}(t_1) \cdots \tilde{v}(t_n) f \, dt_n \cdots dt_1 \quad (296)$$

The first try one might make for showing that $\tilde{u}_{12}$ is Hilbert-Schmidt is to prove that $M_2 \equiv \sup_t \|\tilde{v}(t)\|_{\mathscr{I}_2} < \infty$ for then the nth term in (296) would be Hilbert-Schmidt with Hilbert-Schmidt norm bounded by $|t_0 + t|^n M_2^n/n!$. Unfortunately, M_2 is infinite since

$$\tilde{v}(t) = \begin{pmatrix} e^{iBt}Re^{-iBt} & e^{+iBt}Re^{iBt} \\ -e^{-iBt}Re^{-iBt} & -e^{-iBt}Re^{iBt} \end{pmatrix}$$

where $R = -\frac{1}{2}B^{-1/2}V(x, t)B^{-1/2}$, so

$$\mathrm{Tr}(R^*R) = \tfrac{1}{4} \int |\hat{V}(k - p, t)|^2 (k^2 + m^2)^{-1/2}(p^2 + m^2)^{-1/2} \, d^3k \, d^3p$$

is infinite since the integrand falls only as $|k + p|^{-2}$ as $|k + p| \to \infty$ with $k - p$ fixed. However

$$M_4 \equiv \sup_t \|\tilde{v}(t)\|_{\mathscr{I}_4} < \infty$$

since $|V(x, t)|^{1/2}B^{-1/2}$ is in $\mathscr{I}_8$ by Theorem XI.20 and the fact that $f(y) = (y^2 + m^2)^{-1/4} \in L^8(\mathbb{R}^3)$. Since $\|AB\|_{\mathscr{I}_2} \leq \|A\|_4 \|B\|_4$, the nth term on the right of (296) for $n \geq 2$ is Hilbert-Schmidt with Hilbert-Schmidt norm bounded by $M_4^n |t_0 + t|^n/n!$ Thus since the $n = 0$ term has no 12 element, it suffices to prove that

$$G(t) = \int_{-t_0}^{t} \tilde{v}_{12}(s) \, ds$$

is Hilbert-Schmidt (this would *not* be true if we replaced 12 by 11). Now, $G(t)$ has p-space integral kernel

$$g(k, p, t) = \int_{-t_0}^{t} (k^2 + m^2)^{-1/4}(p^2 + m^2)^{-1/4} \hat{V}(k - p, s) \times \exp[-is(\sqrt{k^2 + m^2} + \sqrt{p^2 + m^2})] \, ds$$

and an integration by parts easily shows that

$$|g(k, p, t)| \leq C[(k^2 + m^2)^{-1/4}(p^2 + m^2)^{-1/4}\{(k^2 + m^2)^{1/2} + (p^2 + m^2)^{1/2}\}^{-1}(1 + |k - p|^2)^{-4}] \quad (297)$$

Thus $g \in L^2(\mathbb{R}^6)$ for each t so $G(t)$ is Hilbert-Schmidt. ∎

This calculation has an intriguing feature when done in four space dimensions. Then (297) is not in L^2, so it is natural to attempt to integrate by parts again. If there is no boundary term from the first integration by parts, then one can improve the falloff and thereby control the $n = 1$ term in (296); but if the boundary term is nonzero, the $n = 1$ term will *not* be Hilbert-Schmidt. For all t, the $n \geq 3$ terms are Hilbert-Schmidt by a direct argument since in this case $M_6 < \infty$, and the $n = 2$ term is Hilbert-Schmidt using a single integration by parts. Since $\hat{V}(\cdot, -t_0) = 0$, the boundary term is not in L^2 if $\hat{V}(\cdot, t) \neq 0$ and therefore we have that in the four space dimensional case, $u_{12}(t, -t_0)$ is Hilbert-Schmidt only for those t with $V(\cdot, t) = 0$. Thus, it can happen that the S-operator *is* unitarily implementable in cases where the dynamics is not implementable for intermediate times. This phenomenon also takes place in three space dimensions if one considers suitable higher spin equations or uses coupling different from that in (278).

We summarize:

Theorem XI.107 Assume that $V(x, t)$ is C^∞ with compact support in $\mathbb{R}^4$. Let φ_{in} be the free charged scalar field of mass m. Then there exist operator-valued distributions $\varphi(x, t)$, $\pi(x, t)$ for each t so that $\pi(x, t) = d\varphi(x, t)/dt$ and (289) holds. There exists a family of unitary operators $U(t, -t_0)$ on $\mathscr{H}$ so that

$$\varphi(x, t) = U(t, -t_0)\varphi_{\text{in}}(x, -t_0)U(t, -t_0)^{-1}$$
$$\pi(x, t) = U(t, -t_0)\pi_{\text{in}}(x, -t_0)U(t, -t_0)^{-1}$$

Finally, let φ_{out} be as defined above. Then there exists a unitary scattering operator S on $\mathscr{H}$ so that

$$\varphi_{\text{out}}(x, 0) = S^{-1}\varphi_{\text{in}}(x, 0)S$$
$$\pi_{\text{out}}(x, 0) = S^{-1}\varphi_{\text{out}}(x, 0)S$$

Finally we note that by extending the ideas above one can prove the following abstract result.

Theorem XI.108 Let $\mathscr{H}$ be a separable complex Hilbert space and let $\mathscr{F}_s(\mathscr{H})$ be the boson Fock space over $\mathscr{H}$. For each $f \in \mathscr{H}$, let $a^-(f)$ be the annihilation operator on $\mathscr{F}_s(\mathscr{H})$ defined by (X.62) and set

$$a(f) = a^-(Cf), \qquad a^\dagger(f) = (a^-(f))^*$$

where C is a fixed conjugation on $\mathscr{H}$. Let $\langle B_+, B_- \rangle$ be a pair of bounded linear transformations on $\mathscr{H}$ that satisfy:

$$B_+^* B_+ - B_-^* B_- = I, \qquad B_+^* C B_- = B_-^* C B_+ \tag{298}$$

$$K_+^* K_+ - K_-^* K_- = I, \qquad K_+^* C K_- = K_-^* C K_+ \tag{299}$$

where

$$K_+ = B_+^*, \qquad K_- = -C B_-^* C \tag{300}$$

and set

$$\begin{aligned} a_B(f) &\equiv a^\dagger(CB_- Cf) + a(CB_+ Cf) \\ a_B^\dagger(f) &\equiv a^\dagger(B_+ f) + a(B_- f) \end{aligned} \tag{301}$$

Then there exists a unitary operator W on $\mathscr{F}_s(\mathscr{H})$ so that

$$\begin{aligned} a_B(f) &= W^{-1} a(f) W \\ a_B^\dagger(f) &= W^{-1} a^\dagger(f) W \end{aligned}$$

if and only if B_- is Hilbert-Schmidt. W is uniquely determined up to an overall phase factor.

The mapping $\langle a, a^\dagger \rangle \mapsto \langle a_B, a_B^\dagger \rangle$ given by (301) is called a **Bogoliubov transformation**. The conditions on B_+, B_- are just those needed so that

$$[a_B(f), a_B(g)] = 0 = [a_B^\dagger(f), a_B^\dagger(g)]$$

and

$$[a_B(f), a_B^\dagger(g)] = (Cf, g)_{\mathscr{H}}$$

The K's are the B's for the inverse Bogoliubov transformation and the formulas (299) guarantee invertibility. That is, if (298) and (299) hold, then

$$\begin{aligned} a^\dagger(f) &= a_B^\dagger(K_+ f) + a_B(K_- f) \\ a(f) &= a_B^\dagger(CK_- Cf) + a_B(CK_+ Cf) \end{aligned}$$

XI.16 Quantum field scattering II: The Haag–Ruelle theory

In this section we want to describe scattering ideas in a class of field theories obeying the Wightman axioms of Section IX.8. The free field of Section X.7 will play an important role. In the preceding section we discussed a simple example where the field equation was linear, the interaction was a classical rather than an operator-valued field, and the interaction had compact support in space and time. Even in that case, the construction was nontrivial. How can we hope to construct a scattering theory for a general quantum field theory where none of the above simplifications hold true? The answer is simple. Our construction is axiomatic. We shall assume that the Gårding–Wightman axioms hold; in particular, we assume the existence of a unitary interacting dynamics. It was precisely the construction of such a dynamics that occupied us in the preceding section. Nevertheless, it is striking that the spectrum condition and microcausality conspire in such a way that a scattering theory can be constructed.

The first conceptual problem that must be faced is that there is no natural "free" dynamics for the interacting dynamics to approach as $t \to \pm\infty$. This is of course true in a general axiomatic framework, but it is also true in the types of models introduced in Section X.7 obtained from perturbation of the free field of mass m_0. This is somewhat surprising since one might think that the Hamiltonian H_0 of this free field would play the role of free dynamics. In the first place, the two Hamiltonians act on two different Hilbert spaces for the following reason: When the space cutoff of Section X.7 is removed, one must pass to a new representation of the canonical commutation relations since there is a general result known as Haag's theorem. This theorem asserts that any Wightman field theory in which there are time zero φ's and π's that are unitarily equivalent to those of the free field is the free field theory. Physically significant is the fact that the mass of particles in the interacting theory may not equal m_0; that is, in interacting quantum field theory, unlike classical field theories, the particles can never completely escape their own interaction. These two reasons are connected since, even for the free field, a change in mass means a change in representation of the canonical commutation relations.

In a sense which we shall make precise, the "free dynamics" will be a free field but with the correct physical mass rather than the mass m_0. In this sense there is a similarity to spin-wave scattering in that the comparison dynamics is determined by a piece of the interacting dynamics. The fact that this free field Hamiltonian and the interacting Hamiltonian are naturally

given on different Hilbert spaces will be accommodated by the two Hilbert space formalism. However, looking at the Hamiltonians alone is not really satisfactory. For the mass hyperboloid $\{p \mid p \cdot p = m^2\}$ produces absolutely continuous spectrum of infinite multiplicity on $[m, \infty)$. Thus, by looking only at the spectrum of H, one cannot distinguish whether just the hyperboloid is present or whether there are also "multiparticle states." This situation is somewhat improved by looking at the joint energy-momentum spectrum. But the true scattering theory must be connected with the x space behavior of the field $A(x)$ (to avoid confusion, we use Φ for the free field and A for the interacting field).

As a preliminary, let $\Phi_m(x, t)$ be the free field of mass $m > 0$ described in Section X.7. It is clear from (X.84) that for each fixed t, $\Phi_m(\cdot, t)$ and $\dot{\Phi}_m(\cdot, t)$ are operator-valued distributions; the fact that smearing in t is not needed is a special feature of the free field and is not true in general Wightman theories. Let $f(x, t)$ be a regular wave packet for the Klein–Gordon equation $f_{tt} = \Delta f - m^2 f$ of the type defined and discussed in the first appendix to Section 3. Introduce the symbol $\overset{\leftrightarrow}{\partial}_0$ to mean

$$\left(g \overset{\leftrightarrow}{\partial}_0 k\right)(t) \equiv \int \left[g(x, t) \frac{\partial}{\partial t} k(x, t) - k(x, t) \frac{\partial}{\partial t} g(x, t)\right] d^3x$$

which maps pairs of functions of x and t to a function of t. Then $f \overset{\leftrightarrow}{\partial}_0 \Phi_m$ is independent of time since both f and Φ_m obey the Klein–Gordon equation which is second order in time and $f \overset{\leftrightarrow}{\partial}_0 \Phi_m$ is essentially a Wronskian. In fact, if the Fourier transform of f in the spatial variables has the form

$$\hat{f}(p, t) = (2\mu(p))^{-1/2} h(p) e^{-i\mu(p)t} \tag{302a}$$

then

$$f \overset{\leftrightarrow}{\partial}_0 \Phi_m = i \int h(p) a^\dagger(p)\, d^3p \tag{302b}$$

and if

$$\hat{f}(p, t) = (2\mu(p))^{-1/2} h(p) e^{+i\mu(p)t} \tag{302c}$$

then

$$f \overset{\leftrightarrow}{\partial}_0 \Phi_m = -i \int h(-p) a(p)\, d^3p \tag{302d}$$

In particular, (302b) shows that as N runs through 0, 1, ..., and f_i runs through all choices obeying (302a), the vectors

$$\left(f_1 \overset{\leftrightarrow}{\partial}_0 \Phi_m\right)\left(f_2 \overset{\leftrightarrow}{\partial}_0 \Phi_m\right) \cdots \left(f_N \overset{\leftrightarrow}{\partial}_0 \Phi_m\right) \Omega_0$$

run through a total set of $\mathscr{H}_0$, the Hilbert space of the free field.

Suppose that $\langle \mathscr{H}, U, A, D \rangle$ is a Hermitian scalar field obeying the Gårding–Wightman axioms (Properties 1–8 of Section IX.8) and that one has the following two additional properties:

Property 9 (*upper and lower mass gap*) Let P_μ be the generators of the translation subgroup $U(a, I)$ of the Poincaré representation $U(a, \Lambda)$. For some $m > 0$ and some $\varepsilon > 0$, the spectrum of P_μ is contained in

$$\{0\} \cup H_m \cup \bar{V}_{m+\varepsilon, +}$$
$$\equiv \{0\} \cup \{p \mid p^2 = m^2;\, p_0 > 0\} \cup \{p \mid p^2 \geq (m + \varepsilon)^2;\, p_0 > 0\}$$

where $p^2 = p_0^2 - p_1^2 - p_2^2 - p_3^2$. Moreover, the set of vectors $\mathbb{S}$ which are eigenvectors for p^2 with eigenvalue m^2 is nonempty, and there is a cyclic vector for the action of $U(a, I)$ on $\mathbb{S}$.

$\mathbb{S}$ is the family of vectors describing the states of a single spinless particle of mass m. Property 9 ensures that the eigenvalue m^2 is an isolated eigenvalue of P^2.

Property 10 (*coupling of the vacuum to the one particle states*) The spectral weight $d\rho$ for the Källen–Lehmann representation (Theorem IX.34) has the form

$$d\rho(s) = \delta(s - m) + d\tilde{\rho}(s)$$

where $d\tilde{\rho}$ has support in $[m + \varepsilon, \infty)$.

Property 10 essentially says that the vectors $A(f)\psi_0$ where ψ_0 is the vacuum are not all orthogonal to $\mathbb{S}$. For under that condition $d\rho(s) = \alpha\delta(s - m) + d\tilde{\rho}(s)$ with $\alpha \neq 0$. One can then multiply A by a constant so that the new α is 1.

Pick a function h in $C_0^\infty(\mathbb{R})$ so that $h(y)$ is 1 near $y = m^2$ and supp $h \subset (0, m^2 + \varepsilon)$. Define a new operator-valued distribution $B(\mathbf{x}, t)$ by

$$\hat{B}(p) = h(p^2)\hat{A}(p)$$

that is,

$$B(g) = A(Tg) \tag{303}$$

where

$$\widehat{Tg}(p) = h(p^2)\hat{g}(p)$$

Now let $f \in \mathscr{S}(\mathbb{R}^3)$. Then $\hat{f}(\mathbf{p})e^{-ip_0 t}h(p^2)$ is in $\mathscr{S}(\mathbb{R}^4)$, so we can pick g in (303) to have the form $f(\mathbf{x})\,\delta(t - t_0)$, that is, $B(\mathbf{x}, t)$ is a distribution of $\mathbf{x}$ that is smooth in t, and similarly $\dot{B}(\mathbf{x}, t)$ is a distribution in $\mathbf{x}$. In fact, for $f \in \mathscr{S}(\mathbb{R}^3)$, $B(f, t)$ is C^∞ in t. In particular, for any $f \in C^\infty(\mathbb{R}^4)$ with $f(\cdot, t)$ and $\partial_0 f(\cdot, t)$ in $\mathscr{S}(\mathbb{R}^3)$ for each t, we can form $(f\overset{\leftrightarrow}{\partial}_0 B)(t)$. In general, even if f obeys the Klein–Gordon equation, $(f\overset{\leftrightarrow}{\partial}_0 B)(t)$ is not time independent since B does not obey the Klein–Gordon equation but:

Lemma 1 Let f be a regular wave packet for the mass m Klein–Gordon equation. Then $(f\overset{\leftrightarrow}{\partial}_0 B)(t)\psi_0$ is independent of t where ψ_0 is the vacuum for the theory.

Proof In general, $B(x)$ does not obey the Klein–Gordon equation, but $B(x)\psi_0$ does. ∎

By Property 10,

$$\left(\left(f\overset{\leftrightarrow}{\partial}_0 B\right)\psi_0, \left(g\overset{\leftrightarrow}{\partial}_0 B\right)\psi_0\right) = \left(\left(f\overset{\leftrightarrow}{\partial}_0 \Phi_m\right)\Omega_0, \left(g\overset{\leftrightarrow}{\partial}_0 \Phi_m\right)\Omega_0\right) \tag{304}$$

For the left-hand side of (304) can be written in terms of the two point function for A. Since B has built into it a factor of $h(p^2)$, Property 10 says that only the $\delta(s - m)$ term from the spectral weight survives. What is left is then the same thing that would occur if A were equal to Φ_m. Since $\hat{\Phi}_m(p) = h(p^2)\hat{\Phi}_m(p)$, (304) holds.

The main theorem of the Haag–Ruelle theory is the following:

Theorem XI.109 Let A be a Hermitian scalar field theory obeying the Gårding–Wightman axioms (Properties 1–8) and also Properties 9 and 10. Define B as above. Then:

(a) For any regular wave packets $f^{(1)}, \ldots, f^{(n)}$, the limits

$$\lim_{t \to \mp\infty} \left(f^{(1)}\overset{\leftrightarrow}{\partial}_0 B\right)(t) \cdots \left(f^{(n)}\overset{\leftrightarrow}{\partial}_0 B\right)(t)\psi_0 \equiv \eta_{\substack{\text{in} \\ \text{out}}}(f^{(1)}, \ldots, f^{(n)})$$

exist in the norm topology on $\mathscr{H}$ and are independent of the choice of h. Let $\mathscr{H}_{\text{in}}$ and $\mathscr{H}_{\text{out}}$ denote the closed span of the η_{in} and the η_{out}.

(b) $\mathscr{H}_{\text{in}}$ and $\mathscr{H}_{\text{out}}$ are left invariant by the representation U of the Poincaré group.

(c) There are operator-valued distributions φ_{in} on $\mathscr{H}_{\text{in}}$ and φ_{out} on $\mathscr{H}_{\text{out}}$ so that $\langle \mathscr{H}_{\text{in}}, U, \varphi_{\text{in}} \rangle$ and $\langle \mathscr{H}_{\text{out}}, U, \varphi_{\text{out}} \rangle$ are unitarily equivalent to the free field of mass m and so that

$$\eta_{\substack{\text{in} \\ \text{out}}}(f^{(1)}, \ldots, f^{(n)}) = \left(f^{(1)}\overset{\leftrightarrow}{\partial}_0 \varphi_{\substack{\text{in} \\ \text{out}}}\right) \cdots \left(f^{(n)}\overset{\leftrightarrow}{\partial}_0 \varphi_{\substack{\text{in} \\ \text{out}}}\right)\psi_0$$

Before discussing the physical interpretation of this theorem and its proof, we note a mathematical consequence analogous to the spectral implications of the existence of wave operators in ordinary quantum mechanics. Since U restricted to $\mathscr{H}_{\text{in}}$ is unitarily equivalent to the U of the free field, we have:

Corollary 1 In a field theory obeying Properties 1–10, the energy momentum spectrum contains $\{p \,|\, p^2 \geq (2m)^2;\ p_0 > 0\}$.

In particular, one has the striking fact that one cannot construct a Wightman field theory with $\sigma(P) = \{p \,|\, p^2 = m^2,\ p_0 > 0\} \cup \{0\}$!

To help illustrate the scattering theoretic content of Theorem XI.109, one can either attempt to rewrite it in terms of some kind of wave operator or one can attempt to rephrase the usual nonrelativistic framework into a form similar to Theorem XI.109. We follow the former course here and leave the latter to the references in the Notes and problems (Problem 142). Let $f^{(1)}, \ldots, f^{(n)}$ obey (302a). Define a map J from a dense subset of $\mathscr{H}_0$, the Hilbert space for the free field of mass m, to $\mathscr{H}$ by

$$J\left[\prod_{i=1}^{n}\left(f^{(i)}\overset{\leftrightarrow}{\partial}_0 \Phi_m\right)\Omega_0\right] = \prod_{i=1}^{n}\left(f^{(i)}\overset{\leftrightarrow}{\partial}_0 B\right)(t=0)\psi_0$$

J is well defined because a given vector $\psi \in \mathscr{H}_0$ can be written in at most one way as

$$\psi = \prod_{i=1}^{n}\left(f^{(i)}\overset{\leftrightarrow}{\partial}_0 \Phi_m\right)\Omega_0$$

if the $f^{(i)}$ are required to satisfy (302a). It is because of the requirement that J be well defined that we cannot use the more natural formula

$$J\left[\prod_{i=1}^{n}(\Phi_m(g^{(i)}))\,\Omega_0\right] = \left[\prod_{i=1}^{n}A(g^{(i)})\right]\psi_0$$

Let $\mathscr{D}_0$ be the set of vectors of the form $\prod_{i=1}^n (f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m)\Omega_0$ which is total in $\mathscr{H}_0$ by (302b). Then:

Corollary 2 $\Omega^\pm = \text{s-lim}_{t\to\mp\infty} e^{itH}Je^{-itH_0}$ exist and define partial isometries $\mathscr{H}_0 \xrightarrow{\Omega^+} \mathscr{H}_{\text{in}}$ and $\mathscr{H}_0 \xrightarrow{\Omega^-} \mathscr{H}_{\text{out}}$.

Proof Let $e^{-ith_0}f$ be defined by

$$(e^{-ith_0}f)(x, s) = f(x, t + s)$$

Then

$$e^{-itH_0}\left[\prod_{i=1}^n f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m\right]\Omega_0 = \prod_{i=1}^n \left[e^{-ith_0}f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m\right]\Omega_0$$

so

$$e^{itH}Je^{-itH_0}\left[\prod_{i=1}^n f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m\right]\Omega_0 = \prod_{i=1}^n e^{itH}\left(f^{(i)}(\cdot, t)\overleftrightarrow{\partial}_0 B(\cdot, 0)\right)e^{-itH}\psi_0$$
$$= \prod_{i=1}^n \left(f^{(i)}\overleftrightarrow{\partial}_0 B\right)(t)\psi_0$$

so by Theorem XI.109, the limits defining $\Omega^\pm$ exist and

$$\Omega^\pm\left[\prod_{i=1}^n f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m\right]\Omega_0 = \prod_{i=1}^n (f^{(i)}\overleftrightarrow{\partial}_0 \varphi_{\substack{\text{in}\\\text{out}}})\psi_0 \tag{305}$$

By (c) of the theorem, $\Omega^\pm$ are isometries. ∎

(305) says that

$$\Omega^\pm \Phi_m = \varphi|_{\substack{\text{in}\\\text{out}}} \Omega^\pm$$

In particular, the Jauch S-matrix $S = \Omega^+(\Omega^-)^*$ obeys

$$\varphi_{\text{out}} = S^{-1}\varphi_{\text{in}}S$$

if we have the condition of *asymptotic completeness*

$$\mathscr{H}_{\text{in}} = \mathscr{H}_{\text{out}} = \mathscr{H} \tag{306}$$

It certainly happens that (306) fails in some models, for example, in many generalized free fields (see the Notes to Section IX.8). One hopes that this is due to the artificiality of the models and that real models will obey asymptotic completeness, at least if one can construct asymptotic fields for each

discrete mass hyperboloid and build the corresponding states with all possible asymptotic particles. For this reason, in further developments, (306) is often taken as an axiom.

We now turn to the proof of Theorem XI.109. It depends on four facts. The first is Lemma 1; the second is the falloff of regular wave packets for the Klein-Gordon equation as summarized in Theorem XI.17 and its corollary. To describe the third we need to introduce the notion of truncated vacuum expectation value (TVEV).

Definition A **partition** of the ordered set $\langle 1, \ldots, n\rangle$ is a family P of ordered subsets $S_1 = \langle i_1, \ldots, i_{k(1)}\rangle, \ldots, S_\ell = \langle i'_1, \ldots, i'_{k(\ell)}\rangle$ so that $i_1 < \cdots < i_{k(1)}, \ldots, i'_1 < \cdots < i'_{k(\ell)}$ and so that $\bigcup S_j = \langle 1, \ldots, n\rangle$ and $S_j \cap S_q = \varnothing$. $\mathscr{P}_n$ will denote the set of all partitions of $\langle 1, \ldots, n\rangle$.

Definition The **truncated vacuum expectation values** of a Wightman theory are the distributions $\mathscr{W}_{n,T}$ defined in terms of the Wightman distributions $\mathscr{W}_n$ by the relation

$$\mathscr{W}_n(x_1, \ldots, x_n) = \sum_{P\in\mathscr{P}_n} \mathscr{W}_{k(1),T}(x_{i_1}, \ldots, x_{i_{k(1)}}) \cdots \mathscr{W}_{k(\ell),T}(x_{i'_1}, \ldots, x_{i_{k(\ell)}})$$

(307)

Clearly, the $\mathscr{W}_{n,T}$ are defined inductively from (307) since if $\mathscr{W}_{1,T}, \ldots, \mathscr{W}_{n-1,T}$ are defined, then exactly one term on the right of (307), namely the one with $P = \{\langle 1, \ldots, n\rangle\}$ is not previously defined and so is defined by (307). The first few $\mathscr{W}_{n,T}$ are given by

$$\mathscr{W}_{1,T}(x_1) = (\psi_0, \varphi(x_1)\psi_0)$$
$$\mathscr{W}_{2,T}(x_1, x_2) = (\psi_0, \varphi(x_1)\varphi(x_2)\psi_0) - (\psi_0, \varphi(x_1)\psi_0)(\psi_0, \varphi(x_2)\psi_0)$$
$$\mathscr{W}_{3,T}(x_1, x_2, x_3) = \mathscr{W}_3(x_1, x_2, x_3) - \mathscr{W}_1(x_1)\mathscr{W}_2(x_2, x_3) - \mathscr{W}_1(x_2)\mathscr{W}_2(x_1, x_3) - \mathscr{W}_1(x_3)\mathscr{W}_2(x_1, x_2) + 2\mathscr{W}_1(x_1)\mathscr{W}_1(x_2)\mathscr{W}_1(x_3)$$

There are a variety of explicit formulas for $\mathscr{W}_{n,T}$ (see the Notes and Problem 143) but the implicit formulas (307) are all that we shall need. The reason that the $\mathscr{W}_{n,T}$ are natural is the following fact which we will eventually prove: Since $\mathscr{W}_{n,T}$ is translation invariant, we can form $W_{n,T}(\zeta_1, \ldots, \zeta_{n-1})$ as in Section IX.8. Under the spectral hypothesis, Property 9, $\tilde{W}_n$

has support in $\bigtimes_{j=1}^{n-1}(-\bar{V}_{m,+}\cup\{0\})$; $\hat{W}_{n,T}$ has support only in $\bigtimes_{j=1}^{n-1}(-\bar{V}_{m,+})$. In particular, the supports of the Fourier transform of $W_{n,T}(\zeta_1,\ldots,\zeta_{n-1})$ and $W_{n,T}(-\zeta_{n-1},\ldots,-\zeta_1)$ will be disjoint, which will be important.

The third basic fact needed in the proof of Theorem XI.109 is the following:

Theorem XI.110 (cluster property of TVEV) Fix $f\in\mathscr{S}(\mathbb{R}^{4n})$. For $a_1,\ldots,a_n\in\mathbb{R}^3$, let

$$F(a_1,\ldots,a_n)=\int_{\mathbb{R}^{4n}}\mathscr{W}_{n,T}(x_1,\ldots,x_n)f(x_1-a_1,\ldots,x_n-a_n)\,dx_1\cdots dx_n \tag{308}$$

(where a_i is used for $\langle a_i,0\rangle\in\mathbb{R}^4$). Define G by

$$G(\alpha_1,\ldots,\alpha_{n-1})=F(a_1,\ldots,a_n);\qquad \alpha_i=a_{i+1}-a_i$$

Then $G\in\mathscr{S}(\mathbb{R}^{3n-3})$.

The last result required for the proof of Theorem XI.109 is:

Theorem XI.111 Let K be a distribution in $\mathscr{S}'(\mathbb{R}^\nu)$ so that $K*f\in\mathscr{S}(\mathbb{R}^\nu)$ for every $f\in\mathscr{S}(\mathbb{R}^\nu)$. Then, for any N, there is a constant coefficient differential operator $P(D)$, and a continuous function F on $\mathbb{R}$ so that

$$K=P(D)F$$
$$|F(x)|\le C(1+x^2)^{-N}$$

We turn now to the proof of Theorem XI.109. Theorems XI.110 and XI.111 are proven later in the section.

Proof of Theorem XI.109 Introduce the symbol $B_f(t)$ for $f(\cdot,t)\overleftrightarrow{\partial}_0 B(\cdot,t)$. Let $C_1(t),\ldots,C_n(t)$ be n operators each of which is either a $B_f(t)$ or a time derivative of a $B_f(t)$. Let $(\psi_0,C_1(t)\cdots C_n(t)\psi_0)_T$ denote a truncated expectation as defined above. We first claim that

$$|(\psi_0,C_1(t)\cdots C_n(t)\psi_0)_T|\le c(1+|t|)^{-\frac{1}{2}(n-2)} \tag{309}$$

To prove (309), we first expand the C's as sums of $B(x,t)$'s smeared with f's. The new f's are all regular wave packets for the Klein–Gordon equation since they are the original f's or their time derivatives. Thus the left-hand side of (309) is bounded by a sum of terms of the form

$$\left|\int f^{(1)}(x_1,t)\cdots f^{(n)}(x_n,t)(\psi_0,Q_1(x_1,t)\cdots Q_n(x_n,t)\psi_0)_T\,d^{3n}x\right| \tag{310}$$

where each Q is B, $\partial_0 B$ or $\partial_0^2 B$. Define $K(\zeta_1,\ldots,\zeta_{n-1})$ by

$$K(\zeta_1,\ldots,\zeta_{n-1})=(\psi_0,Q_1(x_1,t)\cdots Q_n(x_n,t)\psi_0)_T;\qquad \zeta_i=x_{i+1}-x_i$$

$K\in\mathscr{S}'(\mathbb{R}^{3n-3})$ and is independent of t by the time translation covariance of the theory. By (303), K smeared with a g in $\mathscr{S}(\mathbb{R}^{3n-3})$ can be rewritten as $W_{n,T}$ smeared with a $\tilde{g}$ in $\mathscr{S}(\mathbb{R}^{4n-4})$; so by Theorem XI.110, $K*g\in\mathscr{S}(\mathbb{R}^{3n-3})$ for each g in $\mathscr{S}(\mathbb{R}^{3n-3})$. Thus, by Theorem XI.111, we can find a differential operator $P(D)$ and continuous function F so that $K=P(D)F$ and

$$|F(\zeta_1,\ldots,\zeta_{n-1})|\le C(1+|\zeta|^2)^{-3n}$$

Therefore, (310) can be dominated by a sum of terms of the form

$$C\left|\int g_1(x_1,t)\cdots g_n(x_n,t)(1+|\zeta|^2)^{-3n}\,d^{3n}x\right| \tag{311}$$

where each g_i is a derivative of an $f^{(i)}$ and thus a regular wave packet for the Klein–Gordon equation. As a result, by the corollary to Theorem XI.17,

$$|g_2(x_2,t)|\le c_2(1+|t|)^{-\frac{3}{2}},\ldots,|g_n(x_n,t)|\le c_n(1+|t|)^{-\frac{3}{2}}$$
$$\int|g_1(x_1,t)|d^3x_1\le c_1(1+|t|)^{\frac{3}{2}}$$

so that (311) is dominated by

$$c(1+|t|)^{-\frac{3}{2}(n-1)}\int|g_1(x,t)|(1+|\zeta|^2)^{-3n}\,d^{3n}x\le d(1+|t|)^{-\frac{3}{2}(n-2)}$$

This proves (309).

Using (309), we can prove that the limit in Theorem XI.109 (a) exists by a modified Cook argument. Let

$$\eta(t)=B_{f^{(1)}}(t)\cdots B_{f^{(n)}}(t)\psi_0$$

We shall prove that

$$\left\|\frac{d\eta}{dt}\right\|\le c(1+|t|)^{-\frac{3}{2}} \tag{312}$$

so that $\lim_{t\to\mp\infty}\eta(t)$ exists. Clearly $\|d\eta/dt\|^2$ is a sum of $(\psi_0,C_1(t)\cdots C_{2n}(t)\psi_0)$ terms and thus a sum of products of $(\psi_0,C_{i_1}(t)\cdots C_{i_k}(t)\psi_0)_T$. Since $(\psi_0,B(x,t)\psi_0)=0$, none of the products has one-point TVEV's. Each product is one of the following types:

(1) One of the factors is an m-point TVEV with $m \geq 4$. By (309), this factor is bounded by $(1 + |t|)^{-3}$.
(2) No factor is an m-point TVEV with $m \geq 4$, but at least one three-point TVEV occurs. In this case, since $2n$ is even, at least two such factors must occur, each with $(1 + |t|)^{-3/2}$ falloff, so again the overall falloff is at least $(1 + |t|)^{-3}$.
(3) All the factors are two-point functions. In this case one of the factors must be of the form

$$\left(\psi_0, B_{f^{(1)}}(t)\frac{dB_{f^{(2)}}}{dt}(t)\psi_0\right) \quad \text{or} \quad \left(\psi_0, \frac{dB_{f^{(1)}}(t)}{dt}\frac{dB_{f^{(2)}}(t)}{dt}\psi_0\right)$$

or

$$\left(\psi_0, \frac{dB_{f^{(1)}}}{dt}(t)B_{f^{(2)}}(t)\psi_0\right) = \left(\frac{dB_{\overline{f^{(1)}}}}{dt}(t)\psi_0, B_{f^{(2)}}(t)\psi_0\right)$$

which all vanish, by Lemma 1. Thus such products vanish.

We therefore see that $\|d\eta/dt\|^2 \leq C(1 + |t|)^{-3}$ proving (312) and so part (a) of the theorem.

The invariance of $\mathscr{H}_{\text{in}}$ and $\mathscr{H}_{\text{out}}$ under space–time translations is obvious. The invariance under Lorentz transformations and the independence of the limits of the choice of h are discussed in the references in the Notes.

Motivated by (302), we define $a_{\text{in}}(p)$ and $a_{\text{in}}^\dagger(p)$ by

$$\left(i\int h(p)a_{\text{in}}^\dagger(p)\,d^3p\right)(\eta_{\text{in}}(f^{(2)}, \ldots, f^{(n)})) = \eta_{\text{in}}(f^{(1)}, \ldots, f^{(n)})$$

where h and $f^{(1)}$ are related by (302a) and similarly for $a_{\text{in}}(p)$ using (302c). φ_{in} is then defined using (X.85). The covariance of φ_{in} and φ_{out} under space–time translations is immediate; and, again, the Lorentz covariance can be found in the references. The unitary equivalence of φ_{in} to the free field Φ_m is given by

$$V(\eta_{\text{in}}(f^{(1)}, \ldots, f^{(n)})) = \left[\prod_{i=1}^{n}\left(f^{(i)}\overleftrightarrow{\partial}_0\Phi_m\right)\right]\Omega_0$$

To check that V is well defined and unitary we need only prove that

$$(\eta_{\text{in}}(f^{(1)}, \ldots, f^{(m)}), \eta_{\text{in}}(g^{(1)}, \ldots, g^{(n)})) = \left(\left(\prod_{i=1}^{m} f^{(i)}\overleftrightarrow{\partial}_0\Phi_m\right)\Omega_0, \left(\prod_{i=1}^{n} g^{(i)}\overleftrightarrow{\partial}_0\Phi_m\right)\Omega_0\right) \tag{313}$$

It is then easy to check that

$$V\varphi_{\text{in}}V^{-1} = \Phi_m$$

The left-hand side of (313) is the limit of $(\prod B_{f^{(i)}}\psi_0, \prod B_{g^{(i)}}(t)\psi_0)$ as $t \to -\infty$. Expanding this product as a sum of TVEV's, those terms with some m-point TVEV with $m \geq 3$ vanish by (309). The only terms remaining as $t \to -\infty$ are products of two-point functions which, by Lemma 1, are time independent as we have explained. And, by Property 10, these are identical to the two point function for Φ_m; See (304). Since the n-point function of the free field is a sum of products of two-point functions (see (X.162)), (313) holds. ∎

Proof of Theorem XI.111 By the closed graph theorem $f \mapsto K * f$ is continuous. Let $T = \hat{K}$. Then, by hypothesis and $\widehat{K * f} = (2\pi)^{\nu/2}\hat{K}\hat{f}$ (Theorem IX.4), gT is in $\mathscr{S}(\mathbb{R}^\nu)$ for any $g \in \mathscr{S}(\mathbb{R}^\nu)$. It follows that T is a C^∞ function each of whose derivatives is of polynomial growth, that is, $T \in \mathscr{O}_M$ (see Problem 23 of Chapter V). Given N, pick k so that for all α with $|\alpha| \leq 2N$,

$$|(D^\alpha T)(x)| \leq c(1 + x^2)^k$$

Now let $G(x) = (1 + x^2)^{-k-\nu}T(x)$. Then for $|\alpha| \leq 2N$,

$$|(D^\alpha G)(x)| \leq c(1 + x^2)^{-\nu}$$

Thus since each $D^\alpha G$ is in L^1, $F = \check{G}$ is a distribution which is a bounded continuous function with $x^\alpha F(x)$ bounded for each $|\alpha| \leq 2N$. Therefore

$$|F(x)| \leq c(1 + x^2)^{-N}$$

and $K = (1 - \Delta)^{k+\nu}F$. ∎

We now begin the proof of Theorem XI.110. We first need to establish that $\hat{W}_{n,T}$ has support in $(-\bar{V}_{m,+})^{(n-1)}$.

Lemma 2 Let a be a spacelike vector in $\mathbb{R}^4$. Then

$$\lim_{\lambda\to\infty} \mathscr{W}_n(x_1, \ldots, x_i, x_{i+1} + \lambda a, \ldots, x_n + \lambda a) = \mathscr{W}_i(x_1, \ldots, x_i)\mathscr{W}_{n-i}(x_{i+1}, \ldots, x_n)$$

in the sense that for any $f \in \mathscr{S}(\mathbb{R}^{4i})$, $g \in \mathscr{S}(\mathbb{R}^{4(n-i)})$,

$$\mathscr{W}_n(f \otimes g_\lambda) \to \mathscr{W}_i(f)\mathscr{W}_{n-i}(g) \tag{314}$$

as $\lambda \to \infty$ where

$$(f \otimes g_{\lambda a})(x_1, \ldots, x_n) = f(x_1, \ldots, x_i) g(x_{i+1} - \lambda a, \ldots, x_n - \lambda a)$$

Moreover, the Fourier transform of $W_n(\zeta_1, \ldots, \zeta_{n-1})$ is a (signed) measure in the p_i variable (when smeared in the other variables) and

$$\hat{W}_n(p_1, \ldots, p_{n-1}) = (2\pi)^2 \hat{W}_i(p_1, \ldots, p_{i-1}) \hat{W}_{n-i}(p_{i+1}, \ldots, p_{n-1}) \delta(p_i) + R(p) \tag{315}$$

where, after smearing in the other variables, R is a measure in p_i assigning zero weight to $p_i = 0$.

Proof Fix $f \in \mathscr{S}(\mathbb{R}^{4i})$, $g \in \mathscr{S}(\mathbb{R}^{4(n-i)})$. Let

$$\psi_1 = \int \overline{f(x_1, \ldots, x_i)} \varphi(x_i) \cdots \varphi(x_1) \psi_0 \, dx_1 \cdots dx_i$$

and

$$\psi_2 = \int g(x_1, \ldots, x_{n-i}) \varphi(x_1) \cdots \varphi(x_{n-i}) \psi_0 \, dx_1 \cdots dx_{n-i}$$

Then, as in the proof of Theorem IX.32, if $g_a(x) = g(x_1 - a, \ldots, x_{n-i} - a)$,

$$\mathscr{W}_n(f \otimes g_a) = \int_{\mathbb{R}^4} e^{ik \cdot a} \, d(\psi_1, E_k \psi_2)$$

where E_Ω is the spectral measure for the energy-momentum and $\tilde{k} = \langle k_0, -\mathbf{k} \rangle$. By uniqueness of the vacuum

$$d(\psi_1, E_k \psi_2) = (\psi_1, \psi_0)(\psi_0, \psi_2) \delta(\tilde{k}) + R(\tilde{k})$$

From this, (315) follows immediately. (314), which is not used below, is left to the problems (Problem 145). ∎

Lemma 3 For fields obeying Property 9, $\hat{W}_{n,T}$ has support in $(-\bar{V}_{m,+})^{(n-1)}$, $n \geq 2$.

Proof As in the proof of Theorem IX.32, by Property 9, $\hat{W}_n$ has support in $(\{0\} \cup (-\bar{V}_{m,+}))^{n-1}$. $\hat{W}_{n,T}$ clearly has the same property. Moreover, $\hat{W}_{n,T}$ is a measure in each variable as in Lemma 2. Thus, we need only prove that when smeared in all variables except p_i, $\hat{W}_{n,T}$ has no $\delta(p_i)$ contribution. The proof is by induction on n. For $n = 2$, $W_{2,T}(x) = W_2(x) - W_1^2$ so

$$\hat{W}_{2,T}(p) = \hat{W}_2(p) - (2\pi)^2 \delta(p) W_1^2$$

so, by (315), the $\delta(p)$ contribution to $\hat{W}_{2,T}$ is zero. Now suppose by induction that $\hat{W}_{j,T}$ has support in $(-\bar{V}_{m,+})^{(j-1)}$ for $j = 2, \ldots, n-1$. Fix i and consider

$$\hat{\mathscr{W}}_{n,T} = \hat{\mathscr{W}}_n - \sum_{\substack{P \in \mathscr{P}_n \\ P \neq \{1, \ldots, n\}}} \left(\prod_{S_j \in P} \mathscr{W}_{S_j,T} \right)^{\wedge}$$

Break the sum over $\mathscr{P}_n$ into two pieces. The first is those P's where it never happens that some $k_1 \leq i$ and $k_2 \geq i+1$ are in the same subset $S_j \in P$. Clearly the sum over such P's yields the Fourier transform of $\mathscr{W}_i(x_1, \ldots, x_i) \mathscr{W}_{n-i}(x_{i+1}, \ldots, x_n)$ so the contribution of this sum to $\hat{W}_{n,T}(p)$ precisely cancels the $\delta(p_i)$ part of $\hat{W}_n$. In the second piece of the sum, p_i is a sum of momenta in the $\hat{W}_{S_j,T}$ and thus, by the induction hypothesis, this sum has p_i support in $(-\bar{V}_{m,+})$ (see Problem 146). It follows that $\hat{W}_{n,T}(p)$ has no $\delta(p_i)$ contribution, so its support is in $(-\bar{V}_{m,+})^{(n-1)}$. ∎

Proof of Theorem XI.110 Since the function F of (308) has the property that derivatives of F are again of the same form, we need only show that for any N,

$$\sup_\alpha d(\alpha)^N F(a_1, \ldots, a_n) < \infty \tag{316}$$

where $d(\alpha) = (\sum_{i=1}^{n-1} (a_{i+1} - a_i)^2)^{1/2}$. Clearly, it suffices to show that for any unit vector $\hat{\alpha}$ in $\mathbb{R}^{3n-3}$, (316) holds uniformly for $\alpha/\|\alpha\|$ in some fixed neighborhood of $\hat{\alpha}$. Given $\hat{\alpha}$, we first claim that we can find a partition of $\langle 1, \ldots, n \rangle$ into two sets $I = \{i_1, \ldots, i_k\}$ and $I' = \{i'_1, \ldots, i'_{n-k}\}$ so that if $a_{i+1} - a_i = \hat{\alpha}_i$, then $\|a_j - a_{i'}\| \geq n^{-3/2}$ for all $j \in I$ and $i' \in I'$. This follows from the following argument: Some component of $\hat{\alpha}$, say $\hat{\alpha}_j$, must have length at least $n^{-1/2}$. Consider the n planes in $\mathbb{R}^3$ perpendicular to $a_{j+1} - a_j$ through the a_i. Clearly some pair of adjacent planes must be a distance apart at least $n^{-1}\|a_{j+1} - a_j\| \geq n^{-3/2}$. Take I to be those points on one side of the pair of planes and I' on the other. Pick a neighborhood M about $\hat{\alpha}$ so that if $\alpha/\|\alpha\| \in M$, then for all $j \in I$ and $i' \in I'$,

$$\|a_j - a_{i'}\| \geq \frac{1}{2n^{3/2}} \|\alpha\|$$

Let $\tilde{M} = \{\alpha \neq 0 \mid \alpha/\|\alpha\| \in M\}$. We shall prove that (316) holds for $\alpha \in \tilde{M}$. Since the unit sphere can be covered by finitely many M's, (316) will then follow. Define

$$\mathscr{W}'_{n,T}(x_1, \ldots, x_n) = \mathscr{W}_{n,T}(x_{i_1}, \ldots, x_{i_k}, x_{i'_1}, \ldots, x_{i'_{n-k}})$$

$$\mathscr{W}''_{n,T}(x_1, \ldots, x_n) = \mathscr{W}_{n,T}(x_{i'_1}, \ldots, x_{i'_{n-k}}, x_{i_1}, \ldots, x_{i_k})$$

where we order I and I' so that $i_1 < \cdots i_k$; $i'_1 < \cdots < i'_{n-k}$. We claim that, for any N, and any $g \in \mathscr{S}(\mathbb{R}^{4n})$,

$$\sup_{\alpha \in \tilde{M}} |d^N(\alpha)(\mathscr{W}'_{n,T}(g_a) - \mathscr{W}_{n,T}(g_a))| < \infty \tag{317a}$$

$$\sup_{\alpha \in \tilde{M}} |d^N(\alpha)(\mathscr{W}''_{n,T}(g_a) - \mathscr{W}_{n,T}(g_a))| < \infty \tag{317b}$$

Accepting (317) for the time being, let us prove (316) for $\alpha \in \tilde{M}$. Let S' (respectively, S'') be the support of $\mathscr{W}'$ (respectively, supp $\mathscr{W}''$). If $\langle p_1, \ldots, p_n \rangle \in S'$ (respectively, S''), then by Lemma 3 and Problem 146, $P = \sum_{i \in \alpha} p_i$ lies in $-\bar{V}_{m,+}$ (respectively, $\bar{V}_{m,+}$). Let h be a bounded C^∞ function with bounded derivatives so that $h = 1$ on $-\bar{V}_{m,+}$ and $h = 0$ on $\bar{V}_{m,+}$. Let $g = (h\hat{f})^\vee$. Then $\mathscr{W}''_{n,T}(g_a) = 0$ and $\mathscr{W}'_{n,T}(g_a) = \mathscr{W}'_{n,T}(f_a)$. Thus, by (317), $\sup_{\alpha \in \tilde{M}} |d^N(\alpha)\mathscr{W}'_{n,T}(f_a)| < \infty$. Using (317a) again

$$\sup_{\alpha \in \tilde{M}} |d^N(\alpha)\mathscr{W}_{n,T}(f_a)| < \infty.$$

This proves (316).

Thus, we need only prove (317) to complete the proof. Let $\alpha \in M$ be fixed and let $x \in \mathbb{R}^{4n}$ be such that $\|x\| < d(\alpha)/4n^{3/2}$. Then for any $j \in I$, $i' \in I'$,

$$\begin{aligned} \|x_j - x_{i'}\|^2 &\le 2(\|x_{i'}\|^2 + \|x_j\|^2) \\ &\le 2\|x\|^2 < \tfrac{1}{2}(d(\alpha)/2n^{3/2})^2 \\ &\le \tfrac{1}{2}\|a_j - a_{i'}\|^2 \end{aligned}$$

Letting $\zeta = x_{i'} - x_j \in \mathbb{R}^4$ and $\alpha = a_{i'} - a_j \in \mathbb{R}^3$, we have

$$\zeta_0^2 + \zeta^2 < \tfrac{1}{2}\|\alpha\|^2$$

so

$$(|\zeta_0| + |\zeta|)^2 \le 2\zeta_0^2 + 2|\zeta|^2 < \|\alpha\|^2$$

or

$$|\zeta_0| < \|\alpha\| - \|\zeta\| \le \|\alpha + \zeta\|$$

Thus $\zeta + \alpha$ is spacelike, that is, if $\|x\| < d(\alpha)/4n^{3/2}$, $\alpha \in \tilde{M}$ and $j \in I$, $i' \in I'$, then the $(x + a)_{i'}$ and $(x + a)_j$ are spacelike separated. It follows by local commutativity that for such x,

$$\mathscr{W}'_{n,T}(x + a) = \mathscr{W}_{n,T}(x + a)$$

Thus for any $h_{(a)}$ in C^∞ which is 1 for $\|x\| \ge d(\alpha)/4n^{3/2}$,

$$|\mathscr{W}_{n,T}(g_a) - \mathscr{W}'_{n,T}(g_a)| \le |\mathscr{W}^{(a)}_{n,T}(gh_{(a)})| + |\mathscr{W}^{(a)}_{n,T}(gh_{(a)})| \tag{318}$$

where $\mathscr{W}^{(a)}(x) = \mathscr{W}(x + a)$. We can pick $h_{(a)}$ vanishing on the set of those x with $\|x\| \le d(\alpha)/8n^{3/2}$ and so that for $d(\alpha) \ge 1$, the norms $\|D^\beta h_{(a)}\|$ are uniformly bounded in a. By the regularity theorem for tempered distributions, there is some differential operator $P(D)$ and some continuous function F obeying

$$|F(x)| \le c(1 + x^2)^N$$

so that $\mathscr{W}_{n,T} = P(D)F$. Thus

$$\begin{aligned} |\mathscr{W}^{(a)}_{n,T}(gh_{(a)})| &\le c_0 \int (1 + (x + a)^2)^N |P(D)(gh_{(a)})|\, dx \\ &\le c(1 + a^2)^N \int (1 + x^2)^N |P(D)(gh_{(a)})(x)|\, dx \end{aligned}$$

Because of the falloff of g and the support properties of $h_{(a)}$, the integral above goes to zero faster than any power of $d(\alpha)$. Thus (317a) follows from (318) if we note that, for any α, we can choose a corresponding a satisfying $a^2 \le C\, d(\alpha)^2$, say, by taking $a_1 = 0$. The proof of (317b) is similar. ∎

XI.17 Phase space analysis of scattering and spectral theory

The first step of the proof is to wait. It may take a long time for the particle to move far from the scatterer. We need patience. After all, think how long we had to wait for a proof of asymptotic completeness.

V. Enss

In this section we describe a remarkable approach to studying the basic completeness and spectral problems for Schrödinger operators. The method has potentialities for multiparticle systems. We present the two-body problem where, modulo some logarythmic differences in hypotheses, the results for local potentials are very similar to the Agmon–Kato–Kuroda theorem (Theorem XIII.33) proven in Section XIII.8. The methods, however, are strikingly different: the latter theory depends on considerable, albeit elegant, machinery, including restricting Fourier transforms to spheres (Section IX.9), the theory of locally smooth perturbations (Section XIII.7), and the analytic Fredholm theory (Section VI.5). In comparison, this section will use little more than Cook's method, integration by parts (in the context of Theorem XI.14), and one critical piece of physical insight: any state that is not bound will have to spend long times away from the scatterer (this is made precise by the RAGE theorem which we prove in an appendix to this

section) and at those times the potential should be negligible. If we decompose the state at that time into two pieces, one with velocities pointing away from the scattering center and one pointing toward the scattering center, then one piece should not interact appreciably in the future, and the other should not interact appreciably in the past.

Throughout our discussion of the two-body problem we let $H_0 = -\frac{1}{2}\Delta$. This choice of $m = 1$ is convenient since velocities are then identical to momenta. We let $F(S)$ denote the operator that is multiplication by the characteristic function of S.

Definition A symmetric operator V on $L^2(\mathbb{R}^\nu)$ is said to be an **Enss potential** if and only if

(a) V is a relatively bounded perturbation of H_0 with relative bound $a < 1$.
(b) The function h on $[0, \infty)$ given by

$$h(R) = \|V(H_0 + i)^{-1}F(|x| \geq R)\|$$

is in $L^1(0, \infty; dR)$. $h(R)$ is automatically monotone decreasing so

$$\lim_{R\to\infty} h(R) = 0$$

Notice that we do not require V to be a multiplication operator; but if V is such an operator, one can show (Problem 151d) that $h(R)$ is in L^1 if and only if

$$h(R) = \|F(|x| \geq R)V(H_0 + i)^{-1}\|$$

is in L^1. In particular, if V is a multiplication operator with $(1 + |x|)^{1+\varepsilon}V(H_0 + i)^{-1}$ bounded and if V has H_0-relative bound smaller than 1, then V is an Enss potential.

To show how natural the Enss condition is let us begin by showing that if V is an Enss potential, then the wave operators exist. Let f be a function in $\mathscr{S}(\mathbb{R}^\nu)$ such that $\hat{f}$ has compact support in $\{k \,|\, |k| > a\}$. By the corollary to Theorem XI.14

$$|(e^{-itH_0}(H_0 + i)f)(x)| \leq C(1 + |x| + |t|)^{-\nu-1}, \qquad |x| \leq \tfrac{1}{2}a|t|$$

for some C, from which we see that

$$\int_{-\infty}^{\infty} \|F(|x| \leq \tfrac{1}{2}a|t|)e^{-itH_0}(H_0 + i)f\|\, dt < \infty \tag{319}$$

Now write

$$\begin{aligned} Ve^{-itH_0}f = {} & V(H_0 + i)^{-1}F(|x| \leq \tfrac{1}{2}a|t|)e^{-itH_0}(H_0 + i)f \\ & + V(H_0 + i)^{-1}F(|x| \geq \tfrac{1}{2}a|t|)e^{iH_0t}(H_0 + i)f \end{aligned}$$

Then,

$$\begin{aligned} \|Ve^{-itH_0}f\| \leq {} & \|V(H_0 + i)^{-1}\|\,\|F(|x| \leq \tfrac{1}{2}a|t|)e^{-itH_0}(H_0 + i)f\| \\ & + \|V(H_0 + i)^{-1}F(|x| \geq \tfrac{1}{2}a|t|)\|\,\|(H_0 + i)f\| \end{aligned} \tag{320}$$

By (319) the first term is in $L^1(\mathbb{R}, dt)$. By the Enss condition the second term is in $L^1(\mathbb{R}, dt)$, so

$$\int_{-\infty}^{\infty} \|Ve^{-itH_0}f\, dt\| < \infty.$$

and therefore, by the usual density argument and Cook's method, the wave operators $\Omega^\pm(H, H_0)$ exist. In fact, one can say much more. For the two-body case, the basic result is:

Theorem XI.112 (Enss's theorem) Let V be an Enss potential and let $H = H_0 + V$ as a self-adjoint operator sum. Then:

(1) $\Omega^\pm(H, H_0)$ exist and are complete.
(2) $\sigma_{\text{sing}}(H)$ is empty.
(3) The only possible (finite) accumulation point for $\sigma_{\text{pp}}(H)$ is 0 and any nonzero eigenvalue has finite multiplicity.

We remark that, in particular, the results of the theorem imply that $\sigma_{\text{ess}}(H) = [0, \infty)$. This conclusion is not automatic from Weyl's theorem (Section XIII.4) since the operator V may not be relatively compact.

The proof of Enss's theorem requires:

Theorem XI.113 Let $H = H_0 + V$ where $H_0 = -\frac{1}{2}\Delta$ and V is an Enss potential. Let φ_n be a sequence of unit vectors so that:

(i) $\lim_{n\to\infty} \|F(|x| \leq n)\varphi_n\| = 0$.
(ii) For some $a > 0$, $b > 0$,

$$\lim_{n\to\infty} \|[E_{(-a,a)}(H) + E_{(b,\infty)}(H)]\varphi_n\| = 0$$

where $E_\Omega(H)$ is the family of spectral projections for H.

Then $\varphi_n = \varphi_{n;\,\mathrm{in}} + \varphi_{n;\,\mathrm{out}} + \varphi_{n;\,\mathrm{w}}$ where

$$\overline{\lim}\|\varphi_{n;\,\mathrm{in}}\| < \infty, \qquad \overline{\lim}\|\varphi_{n;\,\mathrm{out}}\| < \infty \tag{321}$$

$$\lim_{n\to\infty} \|(\Omega^+ - 1)\varphi_{n;\,\mathrm{in}}\| = 0 = \lim_{n\to\infty} \|(\Omega^- - 1)\varphi_{n;\,\mathrm{out}}\| \tag{322}$$

$$\lim_{n\to\infty} \sup_{t<0} \|F(|x| \le \delta n)e^{-itH_0}\varphi_{n;\,\mathrm{in}}\| = 0 \tag{323}$$

for some $\delta > 0$, and

$$\lim_{n\to\infty} \|\varphi_{n;\,\mathrm{w}}\| = 0 \tag{324}$$

The basic idea will be to decompose φ_n into pieces, one with momenta pointing outward, the other inward. Along the way we shall have left over pieces which we consign to the wastebasket and lump together as $\varphi_{n;\,\mathrm{w}}$. Of course we could retrieve these pieces from the wastebasket and lump them in with $\varphi_{n;\,\mathrm{in}}$ without affecting (321)–(323), but it is conceptually convenient not to do so. We defer the proof of Theorem XI.113 and first use it to prove Theorem XI.112.

Proof of Theorem XI.112 We have already shown that the wave operators exist. Let $\varphi \in \mathscr{H}_{\mathrm{sing}}(H)$ with $E_{(-a,a)}(H)\varphi = E_{(b,\infty)}(H)\varphi = 0$ for some a, b. Since $(H_0 + i)(H + i)^{-1}$ is bounded and $F(|x| \le n)(H_0 + i)^{-1}$ is compact, we see that $F(|x| \le n)(H + i)^{-1}$ is compact. Thus, by the RAGE theorem, proven in the appendix, we can pick τ_n inductively so that $\tau_{n+1} > \tau_n > 0$ and $\|F(|x| \le n)e^{-i\tau_n H}\varphi\| \le 1/n$. Let $\varphi_n = e^{-i\tau_n H}\varphi$. Then φ_n obeys the hypotheses of Theorem XI.113 so

$$\|\varphi_n - \Omega^+\varphi_{n;\,\mathrm{in}} - \Omega^-\varphi_{n;\,\mathrm{out}}\| \to 0 \tag{325}$$

Since Ran $\Omega^\pm \subset \mathscr{H}_{\mathrm{ac}}(H) \subset \mathscr{H}_{\mathrm{sing}}^\perp$, and $\mathscr{H}_{\mathrm{sing}}$ is left invariant by e^{-itH}, we see that $\|\varphi_n\| \to 0$, so $\varphi = 0$. It follows that $\mathscr{H}_{\mathrm{sing}}(H) = \{0\}$.

Next let $\varphi \in \mathscr{H}_{\mathrm{ac}}(H)$ and suppose that $\varphi \in (\mathrm{Ran}\,\Omega^-)^\perp$ and $E_{(-a,a)}(H)\varphi = E_{(b,\infty)}(H)\varphi = 0$ for some a, b. As above, (325) holds. We have that $(\varphi_n, \Omega^-\varphi_{n;\,\mathrm{out}}) = 0$ since e^{-itH} leaves $(\mathrm{Ran}\,\Omega^-)^\perp$ invariant. Moreover,

$$\begin{aligned}
|(\varphi_n, \Omega^+\varphi_{n;\,\mathrm{in}})| &= |(\varphi, e^{i\tau_n H}\Omega^+\varphi_{n;\,\mathrm{in}})| \\
&= |((\Omega^+)^*\varphi, e^{i\tau_n H_0}\varphi_{n;\,\mathrm{in}})| \\
&\le \|F(|x| \ge \delta n)(\Omega^+)^*\varphi\|\,\|\varphi_{n;\,\mathrm{in}}\| \\
&\quad + \|\varphi\|\,\|F(|x| \le \delta n)e^{i\tau_n H_0}\varphi_{n;\,\mathrm{in}}\|
\end{aligned}$$

By (321) the first term goes to zero, and by (323) the second does also. Thus, φ_n is asymptotically orthogonal to $\Omega^+\varphi_{n;\,\mathrm{in}} + \Omega^-\varphi_{n;\,\mathrm{out}}$ and so to itself. It follows that $\varphi = 0$, so $(\mathrm{Ran}\,\Omega^-)^\perp \cap \mathscr{H}_{\mathrm{ac}}(H) = \{0\}$. Thus $\mathrm{Ran}\,\Omega^- = \mathscr{H}_{\mathrm{ac}}(H)$ and similarly $\mathrm{Ran}\,\Omega^+ = \mathscr{H}_{\mathrm{ac}}(H)$, so the wave operators are complete.

Finally, suppose that φ_n is a sequence of orthogonal normalized eigenvectors of H, $H\varphi_n = E_n\varphi_n$ and $E_n \to E \neq 0$. If we choose a, b with $E \notin [-a, a] \cup [b, \infty)$, then hypothesis (b) of Theorem XI.113 holds. Moreover, by the compactness of $F(|x| \le R)(H + i)^{-1}$, and the orthonormality of $\{\varphi_n\}$, we have that

$$\|F(|x| \le R)\varphi_n\| = |E_n + i|\,\|F(|x| \le R)(H + i)^{-1}\varphi_n\| \to 0$$

By passing to a subsequence we see that we can suppose that the φ_n obey hypothesis (a) of Theorem XI.113. Thus (325) holds, so that φ_n is asymptotically in $\mathscr{H}_{\mathrm{ac}}(H)$ which is impossible. This contradiction implies that conclusion (3) is valid. ∎

The proof of Theorem XI.113 depends on three preparatory lemmas. The first is an argument that we shall repeat in Section XIII.5 that says that H and H_0 look alike at large distances:

Lemma 1 Let Φ be a continuous function on $\mathbb{R}$ vanishing at infinity. Then

$$\lim_{n\to\infty} \|[\Phi(H) - \Phi(H_0)]F(|x| \ge n)\| = 0 \tag{326}$$

Proof Since H is bounded from below, choose $E_0 < \inf \sigma(H) - 1$. Then, for $z \le E_0 + 1$ and $\Phi(x) = (x - z)^{-1}$, (326) holds since

$$\|[\Phi(H) - \Phi(H_0)]F(|x| \ge n)\| \le \|(H - z)^{-1}\|\,\|V(H_0 - z)^{-1}F(|x| \ge n)\|$$

and the second factor goes to zero by the Enss condition and a simple argument (Problem 151c). Since $(H - z)^{-1} - (H_0 - z)^{-1}$ is uniformly bounded and analytic on $\mathrm{Re}\, z \le E_0 + 1$, the Vitali convergence theorem implies convergence of derivatives of $[(H - z)^{-1} - (H_0 - z)^{-1}]F(|x| \ge n)$ to zero, i.e., (326) holds for $\Phi(x) = (x - E_0)^{-m}$ and thus for Φ a polynomial in $(x - E_0)^{-1}$. But, by the Stone–Weierstrass theorem, such polynomials are $\|\cdot\|_\infty$-dense in the continuous functions on $[E_0 + 1, \infty)$ vanishing at infinity. By an $\varepsilon/3$-argument, (326) results for all claimed Φ. ∎

Secondly, we need a slightly refined version of the Corollary to Theorem XI.14.

Lemma 2 Let K be a compact subset of $\mathbb{R}^\nu$ and let $\mathcal{O}$ be an open neighborhood of K. Let $C(x_0, t) = \{x_0 + vt \mid v \in \mathcal{O}\}$ be the "classically allowed region" for particles starting at x_0 with velocities in $\mathcal{O}$. Then, for any ℓ, there is a number μ and constant D so that

$$|e^{-itH_0}u(x)| \leq D(1 + \operatorname{dist}(x, C(x_0, t)))^{-\ell}\|(1 + |x - x_0|^\mu)u\| \quad (327)$$

for all u with $\operatorname{supp} \hat{u} \subset K$ and all $x \notin C(x_0, t)$.

Proof Without loss we can suppose that $x_0 = 0$ since e^{-itH_0} commutes with translations. By a limiting argument, we can suppose that $u \in \mathcal{S}$. By Theorem XI.14 and the arguments in the proof of its corollary, for $\operatorname{supp} \hat{u} \subset K$, $u \in \mathcal{S}$, and $x \notin C(0, t)$:

$$|(e^{-itH_0}u)(x)| \leq D_0(1 + |x| + |t|)^{-\ell} \sum_{|\alpha| \leq \ell} \|D^\alpha \hat{u}\|_\infty$$

(327) follows if we note that by a Sobolev estimate and the Plancherel theorem

$$\sum_{|\alpha| \leq \ell} \|D^\alpha \hat{u}\|_\infty \leq C_0 \sum_{|\alpha| \leq \ell + \nu + 1} \|D^\alpha \hat{u}\|_2 \leq C_1 \|(1 + |x|^{\ell+\nu+1})u\|_2$$

and that

$$|\operatorname{dist}(x, C(0, t))| \leq C(|x| + |t| + 1) \quad (328)$$

For, let $v_\infty = \sup\{|v| \mid v \in \mathcal{O}\}$. Then, either $|x| \leq v_\infty |t|$, in which case $|\operatorname{dist}(x, C(0, t))| \leq 2v_\infty |t|$ or $|x| \geq v_\infty |t|$, in which case

$$|\operatorname{dist}(x, C(0, t))| \leq 2|x|. \quad \blacksquare$$

Finally, we need a lemma about localizations in phase space.

Lemma 3 Let $\mathcal{X}_\alpha$, $\alpha \in \mathbb{Z}^\nu$, be the characteristic function of the unit cube centered at α. Let $f \in \mathcal{S}$ be a fixed positive function and let $f_\alpha \equiv f * \mathcal{X}_\alpha$. Suppose that $\int f\, d^\nu x = 1$. For each $\alpha \in \mathbb{Z}^\nu$, let g_α be a function in $\mathcal{S}$ so that $\sup_\alpha \|(1 - \Delta)^\nu g_\alpha\|_2 < \infty$. Then ($P = -i\nabla$; $X =$ multiplication by x):

(a) $Tu = \sum_\alpha g_\alpha(P) f_\alpha(X) u$ defined a priori on C_0^∞ defines a bounded map from $L^2(\mathbb{R}^\nu)$ to $L^2(\mathbb{R}^\nu)$.

(b) $\|\sum_{|\alpha| \leq \frac{1}{4}R} f_\alpha(X)u\|_2 \leq C[\|F(|x| \leq \frac{7}{8}R)u\|_2 + R^{-1}\|u\|_2]$ for some R-independent constant C.

Proof (a) $\bar{g}_\alpha(P)g_\beta(P)$ is convolution with a function $h_{\alpha\beta}$. We claim that $|h_{\alpha\beta}(x)| \leq C_0(1 + |x|)^{-2\nu}$ for a constant C_0 independent of α and β. This follows from a uniform bound on $\|\bar{g}_\alpha g_\beta\|_1$ and $\|(-\Delta)^\nu \bar{g}_\alpha g_\beta\|_1$, which by Leibnitz's rule follows from the hypotheses on $\|g_\alpha\|_2$ and $\|(-\Delta)^\nu g_\alpha\|_2$. Thus

$$\begin{aligned}
\|Tu\|^2 &= \sum_{\alpha,\beta} \int \overline{u(x)} f_\alpha(x) h_{\alpha\beta}(x - y) f_\beta(y) u(y)\, dx\, dy \\
&\leq C_0 \sum_{\alpha,\beta} \int |u(x)|\, f_\alpha(x)(1 + |x - y|)^{-2\nu} f_\beta(y)|u(y)|\, dx\, dy \\
&= C_0 \int |u(x)|(1 + |x - y|)^{-2\nu}|u(y)|\, dx\, dy \\
&\leq C_1 \|u\|^2
\end{aligned}$$

where we used $\sum_\alpha f_\alpha = 1$ in the second step and Young's inequality in the last.

(b) Using Young's inequality

$$\|[f * F(|x| \leq \tfrac{3}{4}R)]u\| \leq \|v\| + \|w\|$$

where

$$\begin{aligned}
\|v\| &= \|[f * F(|x| \leq \tfrac{3}{4}R)]F(|x| \leq \tfrac{7}{8}R)u\|_2 \\
&\leq \|f * F(|x| \leq \tfrac{3}{4}R)\|_\infty \|F(|x| \leq \tfrac{7}{8}R)u\|_2 \\
&\leq \|f\|_1 \|F(|x| \leq \tfrac{7}{8}R)u\|_2
\end{aligned}$$

and

$$\begin{aligned}
\|w\| &= \|[f * F(|x| \leq \tfrac{3}{4}R)]F(|x| \geq \tfrac{7}{8}R)u\|_2 \\
&\leq \|[f * F(|x| \leq \tfrac{3}{4}R)]F(|x| \geq \tfrac{7}{8}R)\|_\infty \|u\|_2
\end{aligned}$$

For $|y| \geq \frac{7}{8}R$,

$$\begin{aligned}
(f * F(|x| \leq \tfrac{3}{4}R))(y) &= \int_{|x| \leq \frac{1}{4}R} f(y - x)\, dy \\
&= \int_{|x| \leq \frac{1}{4}R} h(y - x)\, dy
\end{aligned}$$

where $h = fF(|x| \geq \frac{1}{8}R)$, since $y \geq \frac{7}{8}R$ and $|x| \leq \frac{3}{4}R$ implies that $|y - x| \geq \frac{1}{8}R$. Thus $\|w\| \leq \|F(|x| \geq \frac{1}{8}R)f\|_1 \|u\|_2$. $\blacksquare$

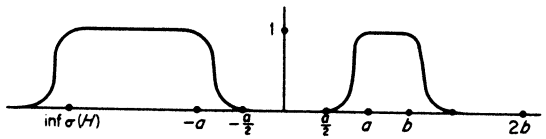


FIGURE XI.16

Proof of Theorem XI.113 Pick a function Φ in $\mathscr{S}(\mathbb{R})$ so that $\Phi = 0$ on $(-\frac{1}{2}a, \frac{1}{2}a)$ and $(2b, \infty)$ and $\Phi = 1$ on $[\inf \sigma(H), -a]$ and $[a, b]$. See Fig. XI.16. Let $\eta_n = \Phi(H_0)\varphi_n$ and

$$\varphi^{(1)}_{n;\,w} \equiv \varphi_n - \eta_n = [1 - \Phi(H)]\varphi_n + [\Phi(H) - \Phi(H_0)]\varphi_n$$

Then $\|\varphi^{(1)}_{n;\,w}\| \to 0$ as $n \to \infty$ since the first term goes to zero by hypothesis (ii) of the theorem and the second term goes to zero by hypothesis (i) and Lemma 1. Moreover, since $\Phi(H_0)$ is convolution with a fixed function in $\mathscr{S}$, we have, as in the proof of part (b) of Lemma 3, that

$$\lim_{n\to\infty} \|F(|x| < \tfrac{7}{8}n)\eta_n\| = 0 \tag{329}$$

We now make the promised decomposition into the piece "going out," and that "going in." Let f be a fixed positive function in $\mathscr{S}(\mathbb{R}^\nu)$ so that $\hat{f}$ has support in $\{k \,|\, |k| < \frac{1}{2}\sqrt{a}\}$ and $\int f(x)\, d^\nu x = 1$. Then $f_\alpha \equiv f * \mathscr{X}_\alpha$ has supp $\hat{f}_\alpha$ also in $\{k \,|\, |k| < \frac{1}{2}\sqrt{a}\}$ and $\widehat{f_\alpha \eta_n}$ has support in $\{k \,|\, \frac{1}{2}\sqrt{a} < |k| < 2\sqrt{b} + \frac{1}{2}\sqrt{a}\}$. Fix functions g and h in $\mathscr{S}$ so that: (i) $g(k) + h(k) = 1$ for $|k| < 2\sqrt{b} + \frac{1}{2}\sqrt{a}$; (ii) $g(k) = 0$ (respectively, $h(k) = 0$) if $|k| > \frac{1}{6}\sqrt{a}$ and k makes an angle of less than 30° with the unit vector in the k_1 (respectively, $-k_1$) direction. Let g_α and h_α be the functions obtained by rotating g and h in such a way that the forbidden cone for g_α (respectively, h_α) is about the direction from α back toward 0 (respectively, the negative of this direction), see Fig. XI.17. We

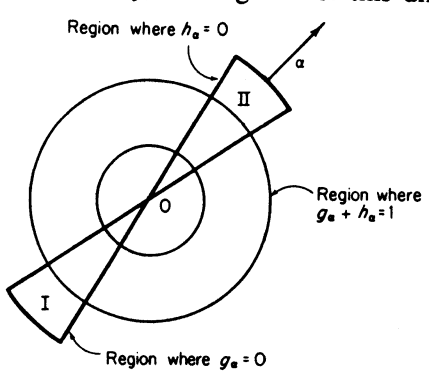


FIGURE XI.17

shall take

$$\varphi_{n;\,\text{in}} = \sum_{|\alpha| \geq \frac{3}{4}n} h_\alpha(P) f_\alpha(X)\eta_n \equiv \sum \eta_{n;\,\alpha,\,\text{in}}$$

$$\varphi_{n;\,\text{out}} = \sum_{|\alpha| \geq \frac{3}{4}n} g_\alpha(P) f_\alpha(X)\eta_n \equiv \sum \eta_{n;\,\alpha,\,\text{out}}$$

$$\varphi^{(2)}_{n;\,w} = \sum_{|\alpha| \leq \frac{3}{4}n} f_\alpha(X)\eta_n; \qquad \varphi_{n;\,w} = \varphi^{(1)}_{n;\,w} + \varphi^{(2)}_{n;\,w}$$

Since supp $\widehat{f_\alpha \eta_n}$ is contained in the set where $g_\alpha + h_\alpha = 1$, $\varphi_{n;\,\text{in}} + \varphi_{n;\,\text{out}} + \varphi^{(2)}_{n;\,w} = \eta_n$. Moreover, $\|\varphi^{(2)}_{n;\,w}\| \to 0$ by part (b) of Lemma 3 and (329). Thus (324) holds, and by part (a) of Lemma 3 so does (321). It remains to show (322) and (323).

We next claim that for some fixed $\delta > 0$, all ℓ, $|\alpha| \geq \frac{3}{4}n$, $t \geq 0$, and $|x| \leq \delta(n + |t|)$,

$$|(e^{-itH_0}(H_0 + i)\eta_{n;\,\alpha;\,\text{out}})(x)| \leq C_\ell(1 + |\alpha| + n + |t|)^{-\ell} \tag{330}$$

Using Lemma 2, this follows from two facts:

(a) $\sup_{n,\,\alpha} \| |x - \alpha|^\mu (H_0 + i) g_\alpha(P) f_\alpha(x)\eta_n \| < \infty$. This follows from the fact that $\| |x - \alpha|^\mu f_\alpha \|_\infty$ is uniformly bounded and that the derivatives of $(k^2 + i)g_\alpha$ are uniformly bounded.

(b) Let $C_\alpha(t) = \{\alpha + vt \,|\, v \in \text{supp } g_\alpha(k) \cap \{\frac{1}{2}\sqrt{a} \leq |k| \leq 2\sqrt{b} + \frac{1}{2}\sqrt{a}\}\}$. Then for x, α, t as above,

$$\text{dist}(x, C_\alpha(t)) \geq \delta(1 + |\alpha| + n + |t|) \tag{331}$$

so long as δ is sufficiently small. (331) asserts that for $t \geq 0$, $|\alpha| \geq \frac{3}{4}n$, $|x_0| \leq \delta n$, $|w| \leq \delta$, and

$$v \in V_0 \equiv \text{supp } g_\alpha \cap \{\tfrac{1}{2}\sqrt{a} < |k| \leq 2\sqrt{b} + \tfrac{1}{2}\sqrt{a}\},$$

we have that $\text{dist}(x_0 + wt, \alpha + vt) \geq c(1 + |\alpha| + n + t)$. Suppose we can show that this distance is always nonzero when α is replaced by $(1 - \varepsilon)\alpha$. Then by shrinking δ we can obtain a lower bound by $2c(1 + |\alpha| + t)$, and using $|\alpha| \geq \frac{3}{4}n$ we obtain the desired estimates. That the distance is nonzero just says that a particle starting at $\alpha - x_0$ with velocity $v - w$ does not hit the origin and this is obvious.

From (330) for exponent $\ell + \nu/2$, one immediately obtains for $t > 0$ and $|\alpha| \geq \frac{3}{4}n$,

$$\|F(|x| \leq \delta n + a\delta|t|)(H_0 + i)e^{-itH_0}\eta_{n;\,\alpha;\,\text{out}}\| \leq C'_\ell(1 + |\alpha| + n + |t|)^{-\ell}$$

and then that for $t \geq 0$

$$\|F(|x| \leq \delta n + a\delta|t|)(H_0 + i)e^{-itH_0}\varphi_{n;\,\text{out}}\| \leq C''_\ell(1 + n + |t|)^{-2} \tag{332}$$

This, the analogue for $t \leq 0$ with out replaced by in, and (320), imply (322). (323) follows by proving the analogue of (332) without the extra factor of $(H_0 + i)$. ∎

Appendix to XI.17: The RAGE theorem

In this appendix we shall prove a theorem of Wiener on the L^2-mean value of the Fourier transform of a measure and a result of similar genre which we call the RAGE theorem because of contributions made to it by Ruelle, Amrein, Georgescu, and Enss.

Recall that a finite (positive) Baire measure μ on a locally compact space X has $\mu(\{x\}) = 0$ for all but countably many x and that $\sum_{x \in X} \mu(\{x\}) \leq \mu(X) < \infty$ so that $\sum_{x \in X} |(\mu(\{x\})|^2$ is a finite number.

Theorem XI.114 (Wiener's theorem) Let μ be a finite Baire measure on $\mathbb{R}$ and let

$$F(t) = \int e^{-ixt}\, d\mu(x)$$

be its Fourier transform (up to a factor of $(2\pi)^{-1/2}$). Then

$$\lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} |F(t)|^2\, dt = \sum_{x \in \mathbb{R}} |\mu(\{x\})|^2 \tag{333}$$

In particular, if μ has no pure points, then the limit is zero.

Proof Using the formula for F and Fubini's theorem (the measure $d\mu \otimes d\mu \otimes (2T)^{-1}\, dt$ on $\mathbb{R} \times \mathbb{R} \times [-T, T]$ is finite):

$$\frac{1}{2T}\int_{-T}^{T} |F(t)|^2\, dt = \int d\mu(x) \int d\mu(y) \frac{1}{2T}\int_{-T}^{T} e^{-i(x-y)t}\, dt$$

$$= \int d\mu(x) H(T, x)$$

where

$$H(T, x) = \int d\mu(y)[T(x - y)]^{-1} \sin(T(x - y))$$

The integrand in H is pointwise bounded by 1 and converges to 0 (respectively, 1) as $T \to \infty$ if $y \neq x$ (respectively, $y = x$). Using the dominated convergence theorem:

$$\lim_{T\to\infty} H(T, x) = \mu(\{x\}) \qquad \text{and} \qquad |H(T, x)| \leq \mu(\mathbb{R})$$

Using the dominated convergence theorem again,

$$\lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} |F(t)|^2\, dt = \int d\mu(x)\, \mu(\{x\}) = \sum_{x \in \mathbb{R}} |\mu(\{x\})|^2. \quad ∎$$

We note that this theorem and its proof extend to show that

$$\frac{1}{2N+1}\sum_{n=-N}^{N} |F(n)|^2 \to \sum_{x \in \mathbb{R}} |\mu(\{x\})|^2$$

and that this in turn implies Theorem VII.14b (which we stated without proof in Volume I); see Problem 148.

Definition Let A be a self-adjoint operator. $P_{\text{cont}}(A)$ denotes the projection onto all vectors φ whose spectral measure has no pure points, i.e., $P_{\text{cont}}(A)$ is the projection onto the orthogonal complement of the eigenvectors of A.

Theorem XI.115 (the RAGE theorem) Let A be a self-adjoint operator and let C be a bounded operator, so that $C(A + i)^{-1}$ is compact. Then:

(a) For all $\varphi \in P_{\text{cont}}(A)\mathscr{H}$:

$$\frac{1}{2T}\int_{-T}^{T} \|Ce^{-itA}\varphi\|^2\, dt \to 0 \tag{334}$$

as $T \to \infty$.

(b) For some $\varepsilon(T) \to 0$ as $T \to \infty$, we have that

$$\frac{1}{2T}\int_{-T}^{T} \|Ce^{-itA}P_{\text{cont}}(A)\varphi\|^2\, dt \leq \varepsilon(T)\|(A + i)\varphi\|^2 \tag{335}$$

for all $\varphi \in D(A)$.

(c) (334) is true if the power 2 is dropped and

$$\frac{1}{2T}\int_{-T}^{T} \|Ce^{-itA}P_{\text{cont}}(A)\varphi\|\, dt \leq \varepsilon(T)^{1/2}\|(A + i)\varphi\| \tag{336}$$

Proof (a) follows by a simple density argument from (b) since $D(A) \cap \text{Ran } P_{\text{cont}}(A)$ is dense in Ran $P_{\text{cont}}(A)$ and

$$\frac{1}{2T}\int_{-T}^{T} \|Ce^{-itA}\varphi\|^2\, dt \le \|C\|^2\|\varphi\|^2 \tag{337}$$

(c) follows from (a), (b), and the Schwarz inequality. By writing

$$\|Ce^{-itA}P_{\text{cont}}(A)\varphi\|^2 = \|C(A+i)^{-1}e^{-itA}P_{\text{cont}}(A)(A+i)\varphi\|^2,$$

we see that it suffices to prove the analog of (335) where C is compact and $\varepsilon(T)\|(A+i)\varphi\|^2$ is replaced by $\varepsilon(T)\|\varphi\|^2$.

For any C and T, let

$$\varepsilon_C(T) = \sup_{\varphi\neq 0} \|\varphi\|^{-2}(2T)^{-1}\int_{-T}^{T}\|Ce^{-itA}P_{\text{cont}}(A)\varphi\|^2\, dt$$

Then by (337)

$$\varepsilon_C(T) \le \|C\|^2$$

and since $\|a+b\|^2 \le 2\|a\|^2 + 2\|b\|^2$:

$$\varepsilon_{C+D}(T) \le 2\varepsilon_C(T) + 2\varepsilon_D(T)$$

Thus, to show that $\varepsilon_C(T)\to 0$ for compact C, it suffices to prove it for finite rank C and thus for a C of rank 1. Since $P_{\text{cont}}(A)$ commutes with e^{-iAt}, we need only show that for $\psi \in \text{Ran } P_{\text{cont}}(A)$ and all φ:

$$\frac{1}{2T}\int_{-T}^{T} |(\psi, e^{-itA}\varphi)|^2\, dt \le \varepsilon(T)\|\varphi\|^2$$

with $\varepsilon(T)\to 0$ as $T\to\infty$.

As in the proof of Lemma 1 before Theorem XI.7, we can pass to a spectral representation, so that

$$(\psi, e^{-itA}\varphi) = \int e^{-itx}h(x)\, d\mu(x)$$

where $d\mu$ is the spectral measure for ψ and $\int |h(x)|^2\, d\mu(x) \le \|\varphi\|^2$. As in the proof of Wiener's theorem:

$$\frac{1}{2T}\int_{-T}^{T} |(\psi, e^{-itA}\varphi)|^2\, dt = \int h(x)\, d\mu(x)\int \overline{h(y)}\frac{\sin((x-y)T)}{(x-y)T}\, d\mu(y)$$

Using the Schwarz inequality,

$$\frac{1}{2T}\int_{-T}^{T} |(\psi, e^{-itA}\varphi)|^2\, dt \le \|\varphi\|^2\,\delta(T)$$

with

$$\delta(T) = \left[\int d\mu(x)\, d\mu(y)\left|\frac{\sin((x-y)T)}{(x-y)T}\right|^2\right]^{1/2}$$

As in the proof of Wiener's theorem, $\delta(T)\to 0$ as $T\to\infty$ since μ has no pure points. ∎

Corollary Let A be a self-adjoint operator on a separable Hilbert space with no point spectrum. Then there exists a sequence $t_n\to\infty$ so that $e^{-it_nA}\to 0$ weakly as $n\to\infty$.

Proof Let $\{\varphi_k\}_{k=1}^{\infty}$ be an orthonormal basis. Then $C = \sum_{k=1}^{\infty} 2^{-k/2}(\varphi_k, \cdot)\varphi_k$ is compact; so by the above proof

$$\frac{1}{2T}\int_{-T}^{T}\|Ce^{-itA}\psi\|^2\, dt \le \varepsilon(T)\|\psi\|^2$$

with $\varepsilon(T)\to 0$. It follows that

$$\frac{1}{2T}\int_{-T}^{T}\left[\sum_{k,m} 2^{-k-m}|(\varphi_k, e^{-itA}\varphi_m)|^2\right] dt \le \varepsilon(T)$$

Since the function, g, in brackets is positive and goes to zero in mean, there must be a sequence $t_n\to\infty$ so that $g(t_n)\to 0$ (clearly there exists T_n with $\varepsilon(T_n)\le 2^{-n}$ and then $t_n \in (\frac{1}{2}T_n, T_n)$ with $g(t_n)\le 4(2^{-n})$). But if the sum goes to zero, each $(\varphi_k, e^{-it_nA}\varphi_m)\to 0$ as $n\to\infty$, which implies the weak convergence. ∎

If A has continuous singular spectrum, it can happen that e^{-itA} does not go to zero weakly as $t\to\infty$ (Problem 149).

In *our* presentation of the Lax–Phillips theory, we proved a priori the absence of singular continuous spectrum. The RAGE theorem ideas allow one to avoid this (see Problem 150).

We conclude this appendix by giving a result of RAGE type that will probably be useful in the discussion of multiparticle scattering.

Theorem XI.116 Let A be self-adjoint operator with empty singular spectrum. Let C and D be two bounded operators with $(A+i)^{-1}C$ and $D(A+i)^{-1}$ compact. Then for any ε, we can find P, a projection onto a *finite* number of eigenvectors for A and a $T\ge 0$ so that, for $t > T$,

$$\|D(A+i)^{-2}e^{-iAt}(1-P)C\| \le \varepsilon$$

Before proving this theorem, let us describe a special case. Suppose that $C = D = F(|x| \leq n)$ and $A = -\Delta + V$ where V is a local Enss potential. This theorem then says that if φ is initially localized in $|x| \leq n$, i.e., $F(|x| \leq n)\varphi = \varphi$, then φ can be broken into two pieces: $P\varphi + (1 - P)\varphi$. $P\varphi$ is a linear combination of specific bound states. The other piece has the property that if we wait long enough, it will "leave the region" and not return, i.e.,

$$\|F(|x| \leq n)e^{-itH}(1 - P)\varphi\| \leq \varepsilon\|(H + i)^2\varphi\| \qquad \text{for all} \quad t > T_0$$

Proof of Theorem XI.116 As in the proof of the RAGE theorem, we need only find T and P so that, for $t > T$,

$$\|Q_1 e^{-itA}(1 - P)Q_2\| \leq \varepsilon$$

where Q_1 and Q_2 are two rank 1 operators. Let P_{ac} be the projection onto the absolutely continuous space for A, let $\varphi_1, \varphi_2, \ldots$ be a labeling of the eigenvectors for A and let P_n be the orthogonal projection onto the span of the vectors $\varphi_1, \ldots, \varphi_n$. Finally, let $P_\infty = \text{s-lim } P_n = 1 - P_{ac}$. By the Riemann–Lebesgue lemma (see Section IX.2) $\|Q_1 e^{-iAt}P_{ac}Q_2\| \to 0$ as $t \to \infty$, so we can choose T so that this norm is less than $\varepsilon/2$ for $t > T$. Since Q_2 has rank 1, $\|(P_\infty - P_n)Q_2\| \to 0$ as $n \to \infty$, so that we can choose n with $\|(P_\infty - P_n)Q_2\| \leq (\varepsilon/2)\|Q_1\|$. Choosing $P = P_n$, we have that for $t > T$,

$$\|Q_1 e^{-iAt}(1 - P)Q_2\| \leq \|Q_1 e^{-iAt}P_{ac}Q_2\| + \|Q_1 e^{-itA}(P_\infty - P_n)Q_2\| \leq \varepsilon \ \blacksquare$$

NOTES

Section XI.1 The geometric ideas mentioned in the third paragraph of the section determine part of the scattering data without any reference to a comparison dynamics: Basically, scattering cross sections do not require anything more than the geometric ideas while time delay does. For further discussion, see the Davies–Simon paper quoted in the notes to Section 4, J. Dollard, "Scattering into cones, I. Potential scattering," *Comm. Math. Phys.* **12** (1969), 193–203; and J. M. Jauch, R. Lavine, and R. G. Newton, "Scattering into cones," *Helv. Phys. Acta* **45** (1972), 325–330. Various authors have given prescriptions for a quantum-mechanical state to be a "scattering state" or to lie in $\mathscr{H}_{ac} \oplus \mathscr{H}_{sing}$ in geometric terms; see D. Ruelle, "A remark on bound states in potential scattering theory," *Nuovo Cimento A* **61** (1969), 655–662; C. Wilcox, "Scattering states and wave operators in the abstract theory of scattering," *J. Functional Analysis* **12** (1973), 257–274; W. Amrein and V. Georgescu, "On the characterization of bound states and scattering states in quantum mechanics," *Helv. Phys. Acta* **46** (1973), 635–658; J. Dollard, "On the definition of scattering subspace in non-relativistic quantum mechanics," *J. Mathematical Phys.* **18** (1977), 229–232 and K. B. Sinha, "On the absolutely and singularly continuous subspaces in scattering theory," *Ann. Inst. H. Poincaré, Sect. A* **26** (1977), 263–277. The ideas of Ruelle are an important ingredient in the work of Enss discussed in Section 17; see that section, its appendix, and its notes.

The S-transformation we have defined, $S = (\Omega^-)^{-1}\Omega^+$, is sometimes called the "EBFM S-matrix" after O. Ekstein, "Theory of time dependent scattering for multichannel processes," *Phys. Rev.* **101** (1956), 880–889; and F. Berezin, L. Faddeev, and R. Minlos, *Proceedings of the Fourth All-Union Mathematical Conference*, Leningrad, 1961. The S'-transformation is called the "Jauch S-matrix" after J. Jauch, "Theory of the scattering operator, I, II," *Helv. Phys. Acta* **31** (1958), 127–158, 661–684. One can express the distinction in quantum scattering by writing two-body scattering in physicists' formal notation. One writes the function $(2\pi)^{-3/2}\psi(\cdot, k)$ of Sections 6 and 7 as $|k, \text{in}\rangle$ and the analogous state, $(2\pi)^{-3/2}\psi(\cdot, -k)$, which describes a state that is asymptotically a plane wave in the future as $|k, \text{out}\rangle$. Finally, write $(2\pi)^{-3/2}e^{ik\cdot x}$ as $|k, \text{free}\rangle$. The quantity of physical interest is $S(k, k') = \langle k, \text{out}|k', \text{in}\rangle$. S and S' are formally given by

$$S(k, k') = \langle k, \text{free}|S|k', \text{free}\rangle$$
$$= \langle k, \text{in}|S'|k', \text{in}\rangle$$

We see explicitly that S and S' are related by the similarity transformation Ω^+: $|k, \text{free}\rangle \mapsto |k, \text{in}\rangle$.

Section XI.2 Much of this section and, in particular, Theorems XI.1, XI.2, and XI.3, are from B. Simon, "Wave operators for classical particle scattering," *Comm. Math. Phys.* **23** (1971), 37–48. Similar results in a different framework have been found by J. Cook, "Banach algebras and asymptotic mechanics," in *Cargese Lectures in Theoretical Physics* (F. Lurchit, ed.) Gordon and Breach, New York, 1967; by W. Hunziker, "The S-matrix in classical mechanics," *Comm. Math. Phys.* **8** (1968), 282–299; and by R. Prosser, "On the asymptotic behavior of certain dynamical systems," *J. Mathematical Phys.* **13** (1972), 186–196. Cook, Hunziker, and Prosser work in the framework of $L^2(\Sigma, d^6x)$ and define unitary operators by $(U_t^{(0)}f)(w) = f(T_t^{(0)}w)$ and $(U_t f)(w) = f(T_t w)$. They then form wave operators as s-$\lim_{t\to\pm\infty} U_{-t}U_t^{(0)}$ using the methods developed in quantum theory. We feel that the treatment directly on phase space is more natural.

The beautiful argument used in Theorem XI.3 to prove that $\mu(N_+ \Delta N_-) = 0$ appeared in J. E. Littlewood, "On the problem of n bodies," *Comm. Sem. Math. Lund*, tome supp. dédié à M. Riesz (1952), 143–151, and C. L. Seigel, *Vorlesungen über Himmelsmechanik*, Springer-Verlag, New York, Heidelberg, Berlin, 1956; it was rediscovered by Hunziker in the reference quoted above. Littlewood also considered some cases with Coulomb forces.

Scattering from central potentials, that is, the formula (7), is discussed and derived in a variety of textbooks; see, for example, L. Landau and E. Lifshitz, *Classical Mechanics*, Pergamon Press, New York, 1960; or R. Newton, *Scattering Theory of Waves and Particles*, McGraw-Hill, New York, 1966.

The use in Theorem XI.3 of the formula $\ddot{I} = \dot{\mathbf{r}}^2 + \mathbf{r} \cdot \mathbf{F}$ is closely connected to the virial theorem (see Landau–Lifshitz). In the central case, its use can be replaced with an application of conservation of energy and of angular momentum (see Problem 14).

Section XI.3 Many of the notions of the abstract time-dependent theory were developed first in the context of two-body quantum systems as described in Section 4. Wave operators were first formalized by C. Møller in "General properties of the characteristic matrix in the theory of elementary particles," I, *Danske. Vid. Selsk. Mat.-Fys. Medd.* **23** (1945), 1–48, who was not

precise about what notion of limit was to be used. K. Friedrichs in "On the perturbation of continuous spectra," *Comm. Pure Appl. Math.* **1** (1948), 361–406, introduced wave operators in a class of models where V is rank one. This paper of Friedrichs also contained ideas germinal to the perturbation theory of embedded eigenvalues as described in Sections XII.5 and XII.6. Friedrich's work remained dormant until the work of Jauch (quoted in the Notes to Section 1), Cook, and Kato (quoted below) in 1957–1958.

Cook's method (Theorem XI.4) appeared in J. Cook, "Convergence of the Moller wave matrix," *J. Math. and Phys.* **36** (1957), 82–87, in the concrete situation, $\mathscr{H} = L^2(\mathbb{R}^3)$, $V \in L^2$, $A = -\Delta + V$; $B = -\Delta$. Theorem XI.5 is an abstraction of the idea of J. Kupsch and W. Sandhas, "Møller operators for scattering on singular potentials," *Comm. Math. Phys.* **2** (1966), 147–154. Until recently, the only way known to treat wave operators when $A - B$ is given as a quadratic form was to rely on more sophisticated and complicated methods than Cook's such as the Kato–Birman theory. A theorem stronger than Theorem XI.6 was proven by M. Schechter, "A new criterion for scattering theory," *Duke Math. J*, **44** (1977), 863–877, who relied on time-independent methods rather than Cook's method. Motivated by Schechter's work, B. Simon in "Scattering theory and quadratic forms: On a theorem of Schechter," *Comm. Math. Phys.* **53** (1977), 151–153, proved Theorem XI.6 as we prove it in the text. This theorem has been extended to the case of two Hilbert space scattering by Schechter in "Wave operators for pairs of spaces and the Klein–Gordon equation," *Aequationes Mathematicae*, to appear.

The Kato–Birman theory has as one of its consequences an invariance theorem for the absolutely continuous spectrum with a hypothesis on the perturbation that is independent of the perturbed operator. A similar kind of theorem exists for the essential spectrum; see Section XIII.4. Unfortunately, no such invariance theorem can exist for the singular continuous spectrum. For it is possible to find a self-adjoint operator A and a rank one perturbation C so that A has no singular continuous spectrum but $A + C$ does. This example is discussed in Section XIII.6. As a result, any invariance theorem for the singular continuous spectrum must make hypotheses that relate the perturbation and the unperturbed operator.

What we have chosen to call the Kato–Birman theory has an involved history. Kato introduced the notion of generalized wave operators and proved that $\Omega^{\pm}(A, B)$ exist and are complete if $A - B$ is finite rank in "On finite dimensional perturbations of self-adjoint operators," *J. Math. Soc. Japan* **9** (1957), 239–249. This was extended to the case $A - B \in \mathscr{I}_1$ with A and B purely absolutely continuous in M. Rosenblum, "Perturbations of continuous spectrum and unitary equivalence," *Pacific J. Math.* **7** (1957), 997–1010; and then to the general trace class case (Theorem XI.8) in T. Kato, "Perturbation of continuous spectra by trace class operators," *Proc. Japan Acad.* **33** (1957), 260–264. These results were proven by basically time-independent methods; a fully time-dependent proof was given by Kato in his book *Perturbation Theory For Linear Operators*, Springer-Verlag, New York, Heidelberg, Berlin, 1966.

The idea of using resolvents to extend the Kato–Rosenblum theorem to cases where $A - B$ is unbounded is due to R. Putnam, "Continuous spectra and unitary equivalence," *Pacific J. Math.* **7** (1957), 993–995. S. Kuroda, in "Perturbations of continuous spectra by unbounded operators, I, II," *J. Math. Soc. Japan* **11** (1959), 247–262; **12** (1960), 243–257, proved a weak version of Theorem XI.9, namely, if $B - A$ is relatively B-bounded and $(A + i)^{-1} = (B + i)^{-1} + (A + i)^{-1}C^*D(B + i)^{-1}$ with both $C(B + i)^{-1}$ and $D(A + i)^{-1}$ Hilbert–Schmidt, then $\Omega^{\pm}(A, B)$ exist and are complete. Theorem XI.9 in case A and B are bounded from below is due to M. Birman, "Conditions for the existence of wave operators," *Dokl. Akad. Nauk SSSR* **143** (1962), 506–509. The general case is due to L. deBranges, "Perturbation of self-adjoint transformations," *Amer. J. Math.* **84** (1962), 543–580; and M. Birman, "A criterion for existence of wave operators," *Izv. Akad. Nauk. SSSR Ser. Mat.* **27** (1963), 883–906.

Theorem XI.10 is due to M. Birman, "A local criterion for the existence of wave operators," *Izv. Akad. Nauk SSSR Ser. Mat.* **32** (1968), 914–942, (English translation: *Math. USSR-Izv.* **2** (1968), 879–906), whose proof is generally regarded as quite difficult.

The original proofs of the Kato–Birman theory were quite a bit more complicated than the one presented in our proof of Theorem XI.7. The basic idea of that proof was hinted at in D. B. Pearson, "General theory of potential scattering with absorption at local singularities," *Helv. Phys. Acta* **47** (1974), 249–264; and, following suggestions by J. Ginibre and T. Kato, presented in D. B. Pearson, "A generalization of Birman's trace theorem," *J. Functional Anal.* **28** (1978), 182–186. Pearson stated the theorem with the extra factor of J—earlier proofs could also extend this way—which led to the unified approach which we present. The proof we give of Theorem XI.9 and the proof in Problem 25 appear to be new. The proof of Theorem XI.10 from this point of view is due to J. Ginibre and D. Pearson and the proof of Theorem XI.13 from this point of view is due to P. Deift, *Classical Scattering Theory with a Trace Condition*, Princeton Series in Physics, Princeton Univ. Press, to appear. The reference for Theorem XI.13 is given in the Notes to Section 10. Theorem XI.12 is due to D. Yafeev, "A remark concerning the theory of scattering for a perturbed polyharmonic operator," *Math. Notes* **15** (1974), 260–265. We follow the proof given by Reed and Simon who rediscovered Yafeev's result in their paper quoted in the notes to Section 10. The part of the conclusion of Theorem XI.12 involving $\Omega^{\pm}(A, B)$ follows directly from Birman's theorem.

The Kato–Birman theory has been extended to certain pairs $\langle A, B\rangle$ where A is self-adjoint but V is only assumed to be such that iB is maximal accretive by E. B. Davies in *Two Channel Hamiltonians and the Optical Model of Nuclear Scattering*, Oxford Univ. Press, preprint, 1978.

The invariance principle, Theorem XI.11, was proven in successively more complicated situations by Birman in the 1962 and 1963 papers quoted above and T. Kato, "Wave operators and unitary equivalence," *Pacific J. Math.* **15** (1965), 171–180.

The general invariance principle (Theorem XI.23) is due to C. Chandler and A. Gibson, "Invariance principle for scattering with long-range (and other) potentials," *Indiana Univ. Math. J.* **25** (1976), 443–460, whose proof we follow. Earlier results were somewhat weaker in that they required $|t|^{\alpha}\|w'(t)\|_2 \in L^1$ for some $\alpha > \frac{1}{2}$ or at least that $\|w(t) - \Omega^{\pm}u\| = O(t^{-1/2})$ as $t \to \mp\infty$. This is not strictly weaker, but is weaker in most practical situations. The early results appeared in L. A. Sakanovich, "The invariance principle for generalized wave operators," *Functional Anal. Appl.* **5** (1971), 49–55; V. B. Matveev, "The invariance principle for generalized wave operators," *Topics Math. Phys.* **5** (1972), 77–85; and *Theoret. and Math. Phys.* **8** (1971), 663–667; and J. A. Donaldson, A. G. Gibson, and R. Hirsh, "On the invariance principle of scattering theory," *J. Functional Analysis* **14** (1973), 131–145. The result of Chandler and Gibson is stated for a slightly larger class of φ's and is applicable to wave operators with modifications for long-range potentials (see Section 9) and for the two Hilbert space theory.

Other general results on invariance of wave operators have been obtained by M. Wollenberg, "The invariance principle for wave operators," *Pacific J. Math.* **59** (1975), 303, and by P. Obermann and M. Wollenberg, "Abel Wave Operators, I: General theory," *Math. Nachr.* (to appear), and "II: Wave operators for functions of operators," *J. Functional Analysis* (to appear). In the latter papers it is shown that if a weaker notion of wave operator is used, the invariance principle *always* holds.

It is not true, in general, that if $\varphi(A) - \varphi(B)$ is trace class, then $\Omega^{\pm}(A, B)$ exist. For example, take $\varphi(x) = x^2$ and $A =$ multiplication by x, $B =$ multiplication by $|x|$ on $L^2(\mathbb{R})$. However, if φ is invertible, this is certainly true and more generally if for each r, there is an admissible function φ_r with $\varphi_r(A) - \varphi_r(B)$ trace class and φ_r one-to-one on $(-r, r)$, then $\Omega^{\pm}(A, B)$ exist and are complete. This result is discussed in the Kato and Deift books quoted above. As a typical

application, one has the following proof of Theorem XI.9: $(A + i)^{-1} - (B + i)^{-1}$ in $\mathscr{I}_1$ implies that $(A + ir)^{-1} - (B + ir)^{-1}$ is in $\mathscr{I}_1$ for all $r \neq 0$, which implies that its real part $\varphi_r(A) - \varphi_r(B)$ is in $\mathscr{I}_1$ where $\varphi_r(x) = \mathrm{Re}(x + ir)^{-1} = x(x^2 + r^2)^{-1}$. This φ_r obeys the hypothesis of the theorem above, so $\Omega^{\pm}(A, B)$ exist and are complete.

Theorem XI.8 fails in a strong way when $A - B$ is only Hilbert-Schmidt for J. von Neumann, in "Charakterisierung des Spectrums eines Integral-Operators," *Actualités Sci. Indust.* **229** (1935), 38-55, proved that, given any self-adjoint B, there is an A with pure point spectrum and $A - B$ Hilbert-Schmidt. This was extended to the trace ideals $\mathscr{I}_p$ with $p > 1$ in S. Kuroda, "On a theorem of Weyl-von Neumann," *Proc. Japan Acad.* **34** (1958), 11-15.

The Kato-Birman theory has been applied to a variety of situations not discussed in the later sections of the book: There are applications to the spectrum of Toeplitz operators in M. Rosenblum, "The absolute continuity of Toeplitz's matrices," *Pacific J. Math.* **10** (1960), 987-996; and to neutron scattering in Y. Shizuta, "On the fundamental equations of spatially independent problems of neutron thermalization theory," *Progr. Theoret. Phys.* **32** (1964), 489-511.

We describe the history of the two Hilbert space scattering theory in more detail in the notes to Section 10. We mention that the kinematics (Propositions 4 and 5) was systematically developed in T. Kato, "Scattering theory with two Hilbert spaces," *J. Functional Analysis* **1** (1967), 342-369, and that Theorem XI.13 is due to A. Belopol'skii and M. Birman, "The existence of wave operators in scattering theory for pairs of spaces," *Izv. Akad. Nauk SSSR Ser. Mat.* **32** (1968) (English translation: *Math. USSR-Izv.* **2** (1968), 1117-1130).

The idea that stationary phase methods are relevant to scattering theory goes back at least to W. Brenig and R. Haag, "General quantum theory of collision processes," *Fortschr. Physik* **7** (1959), 183-242 (English translation: in *Quantum Scattering Theory* (M. Ross, ed.), Indiana Univ. Press, Bloomington, Indiana, 1963). It is used in various works on long-range scattering; see, for example, the paper of Buslaev and Matveev quoted in the Notes to Section 9, and was raised to a high art by L. Hörmander in his paper quoted in the Notes to Section 9. We follow his presentation closely in Theorems XI.14, XI.15, and XI.16. Theorem XI.17 is important in the Haag-Ruelle scattering theory; we describe its history in the Notes to Section 16.

Theorem XI.20 appears in E. Seiler and B. Simon, "Bounds in the Yukawa$_2$ quantum field theory: Upper bound on the pressure, Hamiltonian bound and linear lower bound," *Comm. Math. Phys.* **45** (1975), 99-114. Theorems asserting that $f(X)g(-i\nabla)$ is trace class for suitable f, g go back to W. Stinespring, "A sufficient condition for an integral operator to have a trace," *J. Reine Angew. Math.* **200** (1958), 200-207, whose results allow f to be of the form given in Theorem XI.21 but restrict g severely. Theorem XI.21 is a special case of a result of M. S. Birman and M. Z. Solomjak, "On estimates of singular numbers of integral operators, III," *Vestnik Leningrad Univ. Fiz. Him.* **24** (1969) (Amer. Math. Soc. *Transl.* **2** (1975)). They introduce the norm

$$\|f\|_{\mathrm{BS}} = \sum_{m \in \mathbb{Z}^n} \left(\int_{0 \leq x_i \leq 1} |f(x - m)|^2 \, dx \right)^{1/2}$$

and show that if $\|f\|_{\mathrm{BS}}$ is finite and $g \in L^2_\delta$, then $f(x)g(-i\nabla)$ is trace class. Since it is easy to show that $\|f\|_{\mathrm{BS}} \leq C\|f\|_{L^2}$, their result implies Theorem XI.21. One can actually show (Problem 37) that it suffices that $\|f\|_{\mathrm{BS}}$ and $\|g\|_{\mathrm{BS}}$ be finite. Conversely, if f and g are nonzero, this condition is also necessary; see B. Simon's book "Trace Ideal Methods," London Math. Soc. Lecture Notes, Cambridge Univ. Press, London and New York, 1979. T. Kato has independently proven Theorems XI.20 and XI.21 (unpublished). We follow Kato's proof of Theorem XI.21. Theorem XI.22 is due to M. Cwikel, "Weak type estimates for singular values and the number of bound states of Schrödinger operators," *Ann. of Math.* **106** (1977), 93-102. Earlier B. Simon, "Analysis with weak trace ideals and the number of bound states of Schrödinger operators," *Trans. Amer. Math. Soc.* **224** (1977), 367-380, had proven the result under the stronger hypotheses $g \in L^{q'}_w(\mathbb{R}^n)$, $q' = q/(q-1)$, and $f \in L^{q-\varepsilon} \cap L^{q-\varepsilon}$ for some $\varepsilon > 0$. There is a theorem of the genre of Theorem XI.22 for the case $1 < q < 2$ using norms related to the $\|\cdot\|_{\mathrm{BS}}$ norm; see Simon's book.

The relation $H_{\mathrm{D}}^2 - m^2 = 2m(1 \otimes H_{\mathrm{S}})$ used in the discussion of Example 2 in the third appendix goes back at least as far as M. H. Johnson and B. A. Lippman, "Motion in a constant magnetic field," *Phys. Rev.* **76** (1949), 828-832. The corresponding invariance of scattering is "obvious" to the physicist who thinks in time-independent terms; see the remarks on the invariance principle in the third appendix to Section 8. At first sight it may appear surprising that one can prove that $\Omega^{\pm}(H_{\mathrm{S}}(A), H_{\mathrm{S}}(0))$ exist without any hypotheses on B, using only hypotheses on A. Notice that $B = \mathrm{curl}\, A$ can have less falloff at infinity than A if A oscillates rapidly, so that the aforementioned phenomenon is connected with the ideas of Appendix 2 to Section 8 and the references in the notes to that section. In fact, it should be possible to prove many of the results of Combescure-Ginibre and Schechter quoted in those notes by using the identity $H_{\mathrm{D}}^2 - m^2 = 2m(1 \otimes H_{\mathrm{S}})$.

Section XI.4 Theorem XI.24 was first proven in case $V \in L^2$ by J. Cook in his basic paper quoted in the Notes to the preceding section. The extension to potentials with $|x|^{-1-\varepsilon}$ falloff is due to M. Hack, "On the convergence to the Møller wave operators," *Nuovo Cimento* **9** (1958), 731-733. About the same time, S. Kuroda, "On the existence and the unitarity property of the scattering operator," *Nuovo Cimento* **12** (1959), 431-454, proved a similar result. Extensions to n dimensions are discussed in F. Brownell, "A note on Cook's wave matrix theorem," *Pacific J. Math* **12** (1962), 47-52. For central potentials, an improved result can be found in E. Lundquist, "On the existence of the scattering operator," *Ark. Mat.* **7** (1967), 145-157. Lundquist's results are implied by Theorem XI.31, but he only uses Cook's method. Extensions of Cook's method to include magnetic fields can be found in T. Ikebe and T. Tayoshi, "Wave and scattering operators for second order elliptic operators in $\mathbb{R}^3$," *Publ. Res. Inst. Math. Sci.* Kyoto **A4** (1968), 483-496.

Extensions of the Hack-Cook theorem to study $-\Delta + V$ where V is not necessarily a multiplication operator can be found in K. Jörgens and J. Weidmann, "Zur Existenz der Wellenoperatoren," *Math. Z.* **131** (1973), 141-151; K. Veselić and J. Weidmann, "Existenz der Wellenoperatoren fur eine allgemeine Klasse von Operatoren," *Math. Z.* **134** (1973), 255-274; "Asymptotic estimates of wave functions and the existence of wave operators," *J. Functional Analysis* **17** (1974), 61-77; C. Wilcox, "Scattering states and wave operators in the abstract theory of scattering," *J. Functional Analysis* **12** (1973), 257-274; and A. M. Berthier and P. Collet, "Existence and completeness of the wave operators in scattering theory with momentum dependent potentials," *J. Functional Analysis* **26** (1977), 1-15.

Theorem XI.25 is due to Kupsch and Sandhas in their paper and Theorem XI.26 is essentially in the Schechter paper, both quoted in the Notes to Section 3. Theorem XI.27 is due to J. Avron and I. Herbst, "Spectral and scattering theory of Schrödinger operators related to the Stark effect," *Comm. Math. Phys.* **52** (1977), 239-254. Further discussion of Theorem XI.25 can be found in D. Robinson, "Scattering theory with singular potentials I. The two-body problem," *Ann. Inst. H. Poincaré Sect. A* **21** (1974), 185-216. Theorems of the type of Theorem XI.30 for $n \leq 3$ appeared first in Kuroda's paper quoted above. Theorem XI.31 is due to S. Kuroda, "On a theorem of Green and Lanford," *J. Mathematical Phys.* **3** (1962), 933-935.

The relation $\overline{S\psi(x)} = (S^*\bar{\psi})(x)$ is called "time reversal invariance" because of a fundamental symmetry of the Hamiltonians, which we discuss. Denote the map $\psi \mapsto \bar{\psi}$ by T. T is antilinear and $TH_0 = H_0 T$, $TV = VT$. Thus $Te^{iH_0 t} = e^{-iH_0 t}T$ and $Te^{iHt} = e^{-iHt}T$. Because of this change of sign, T is called time reversal. One sees immediately that $T\Omega^{\pm} = \Omega^{\mp}T$ so that $T(\Omega^-)^*\Omega^+ = (\Omega^+)^*\Omega^- T = [(\Omega^-)^*\Omega^+]^*T$ from which $\overline{S\psi} = S^*\bar{\psi}$ follows. For particles with spin, time reversal is more complicated. The use of time reversal in quantum theory was first emphasized by E. P. Wigner in "Uber die Operation der Zeitumkehr in der Quantenmechanik," *Nachr. Akad. Wiss. Gottingen Math.-Phys. Kl. II* (1931), 546–559.

Theorems of the genre of Theorem XI.32 are due to P. Deift and B. Simon, "On the decoupling of finite singularities from the question of asymptotic completeness in two-body quantum systems," *J. Functional Analysis* **23** (1976), 218–238. Deift and Simon relied on decoupling with Dirichlet boundary conditions (see Section XIII.15) and Feynman path integral estimates. Their results were considerably generalized and extended by M. Combescure and J. Ginibre, "Scattering and local absorption for the Schrödinger operator," *J. Functional Analysis* **29** (1978), 54–73, who used a smooth cutoff J as in the proof we give. Our proof is patterned on theirs. Both papers were motivated by attempts to understand Pearson's example. Pearson's counterexample appeared in D. Pearson, "An example in potential scattering illustrating the breakdown of asymptotic completeness," *Comm. Math. Phys.* **40** (1975), 125–146, where the details of the counterexample may be found. Earlier than Pearson's paper, several examples where Ran $\Omega^+ \neq$ Ran Ω^- existed, but they all involved pathological behavior at ∞; see T. Kato and S. Kuroda, "A remark on the unitarity property of the scattering operator," *Nuovo Cimento* **14** (1959), 1102–1107; and "The abstract theory of scattering," *Rocky Mountain J. Math.* **1** (1971), 127–171.

References for cluster properties appear in the Notes to the next section.

There is an extensive literature on scattering theory for time-dependent potentials: E. Davies, "Time-dependent scattering theory," *Math. Ann.* **210** (1974), 149–162; J. Goldstein, "Temporally inhomogeneous scattering theory," in *Analyse fonctionnelle et applications* (L. Nachbin, ed.), pp. 125–132, Hermann, Paris, 1975; J. Goldstein and C. Monlezun, "Temporally inhomogeneous scattering theory, II; approximation theory and second order equations," *SIAM J. Math. Anal.* **7** (1976), 276–290; J. Hendrickson, "Temporally inhomogeneous scattering theory for modified wave operators," *J. Mathematical Phys.* **16** (1975), 768–771; and "N-body scattering into cones with long-range time-dependent potentials," *J. Mathematical Phys.* **17** (1976), 729–733; J. Howland, "Stationary scattering theory for time-dependent Hamiltonians," *Math. Ann.* **207** (1974), 315–335; A. Inoue, "An example of temporally inhomogeneous scattering," *Proc. Japan Acad.* **49** (1973), 407–410; and "Wave and scattering operators for an evolving system $d/dt - iA(t)$," *J. Math. Soc. Japan* **26** (1974), 608–624; C. Monlezun, "Temporally inhomogeneous scattering theory," *J. Math. Anal. Appl.* **47** (1974), 133–152; E. Schmidt, "On scattering by time-dependent perturbations," *Indiana Univ. Math. J.* **24** (1975), 925–935; K. Yajima, "Scattering theory for Schrödinger equations with potentials periodic in time;" *J. Math. Soc. Japan* **29**, (4), to appear; S. T. Kuroda and H. Morita, "An estimate for solutions of Schrödinger equations with time-dependent potentials and the associated scattering theory," *J. Fac. Sci. Tokyo* **24** (1977), 459–475; and J. Howland, "Scattering theory for Hamiltonians periodic in time," *Indiana Univ. Math. J.* to appear.

Example 3 is discussed in E. B. Davies, "Scattering from infinite sheets," *Proc. Cambridge Philos. Soc.* (to appear) where the details of the argument that Ran $\Omega^+ =$ Ran Ω^- can be found. Davies also proves a result of interest for the physical interpretation of the approximation by scattering from a single site. Explicitly, if $|W(x)| \leq C(1 + |x|)^{-a}$ and

$$V_L(x) = \sum_{n_2, n_3 \in \mathbb{Z}} W(x_1, x_2 - n_2 L, x_3 - n_3 L)$$

then the wave operators $\Omega^{\pm}(-\Delta + V_L, -\Delta)$ converge strongly to $\Omega^{\pm}(-\Delta + W, -\Delta)$ as $L \to \infty$. This result follows from a general convergence theorem (Problem 16).

Example 4 is discussed in E. B. Davies and B. Simon, "Scattering theory for systems with different spatial asymptotics on the left and right," *Comm. Math. Phys.* (to appear). Earlier references for scattering involving potentials $V(x)$ with limits as $x \to +\infty$ or as $x \to -\infty$ but distinct limits include P. Alsholm and T. Kato, "Scattering theory with long range potentials," *Proc. Amer. Math. Soc. Institute on Partial Differential Equations, 1971*, pp. 393–399 (see Remark (4) on p. 394) and S. Ruijsenaars and P. Bongaarts, "Scattering theory for one-dimensional step potentials," *Ann. Inst. H. Poincaré Sect. A* **26** (1977), 1–17. See Section 17 for another approach to completeness in two-body systems.

Section XI.5 For additional discussion of N-body quantum systems, see Sections XI.17, XIII.2, XIII.3, XIII.5, XIII.10, XIII.11, and XIII.13. A brief readable account of many of the elements of the theory and especially of scattering theory may be found in W. Hunziker, *Mathematical Theory of Multi-particle Quantum Systems*, Lectures in Theoretical Physics, Vol. X (A. Barut and W. Britten, eds.); Gordon and Breach, New York, 1968.

Formal elements of N-body scattering from a wave operator point of view and especially channel orthogonality were first discussed by Jauch in the second paper in his series quoted in the notes to Section 1. Hack's theorem (Theorem XI.34) appeared in "Wave operators in multichannel scattering," *Nuovo Cimento Ser. X* **13** (1959), 231–236. An extension of Hack's theorem to potentials with certain local singularities (essentially an n-body analogue of Theorem XI.25) is proven in W. Hunziker, "Time-dependent scattering theory for singular potentials," *Helv. Phys. Acta* **40** (1967), 1052–1062. See also P. Ferrerro, O. de Pazzis, and D. Robinson, "Scattering theory with singular potentials, II. The N-body problem and hard cores," *Ann. Inst. H. Poincaré Sect. A* **21** (1974), 217–232.

The most comprehensive N-body completeness results have been proven, thus far, in case $N = 3$. The basic idea and techniques as well as the earliest results are due to L. Faddeev, *Mathematical Aspects of the Three Body Problem in Quantum Scattering Theory*, Israel Program for Scientific Translation, 1965 (original Russian monograph published by Steklov Institute, 1963). Important technical improvements and extensions of his results are due to L. Thomas, "Asymptotic completeness in two and three particle quantum mechanical scattering," *Ann. Physics* **90** (1975), 127–165; and J. Ginibre and M. Moulin, "Hilbert space approach to the quantum mechanical three body problem," *Ann. Inst. H. Poincaré Sect. A* **21** (1974), 97–145. In particular, Theorem XI.37 is proven in the Ginibre-Moulin paper.

There have been a number of attempts to extend Faddeev's program to N bodies. Analogues of his basic integral equations are due to O. A. Yakubovsky, "On the integral equations in the theory of N-particle scattering," *Soviet J. Nuclear Phys.* **5** (1967), 937–942; and E. Berezin, "Asymptotic behavior of eigenfunctions of Schrödinger's equation for many particles," *Dokl. Akad. Nauk SSSR* (1965) (English translation: *Soviet Math. Dokl.* **6** (1965), 997–1001). Parts of the analysis have been extended by K. Hepp (using Yakubovsky's equations) in "On the quantum mechanical N-body problem," *Helv. Phys. Acta* **42** (1969), 425–458; and by I. Sigal (using Berezin's equations) in "Asymptotic completeness of multiparticle systems," *Dokl. Akad. Nauk SSSR* **204** (1972) (English translation: *Soviet Math. Dokl.* **13** (1972), 756–760). Both analyses are incomplete in that it is required that certain integral equations in certain auxiliary Banach spaces do not have solutions. Faddeev was able to solve this problem and thus finish the analysis in case $N = 3$ by appealing to results on two-body systems. An abstract version of the Faddeev program in the language of the Kato-Kuroda theory of eigenfunction expansions (see the Notes to Section 6) appears in J. Howland, "Abstract stationary theory of multichannel scattering," *J. Functional Anal.* **22** (1976), 250–282.

Asymptotic completeness for certain special multichannel systems with more than three particles has been announced by G. Hagedorn, "Asymptotic completeness for a class of four particle Schrödinger operators," *Bull. Amer. Math. Soc.* **84** (1978), 155–156, and I. Sigal, "On quantum mechanics of many-body systems with dilation analytic potentials," *Bull. Amer. Math. Soc.* **84** (1978), 152–154.

A different approach from Faddeev's has been advocated by P. Deift and B. Simon in "A time dependent approach to the completeness of multiparticle quantum systems," *Comm. Pure Appl. Math.* **30** (1977), 573–583. They prove a kind of analogue to Proposition 3 in Section 3.

Cluster properties of multichannel wave operators and scattering operators were first derived in W. Hunziker, "Cluster properties of multiparticle systems," *J. Mathematical Phys.* **6** (1965), 6–10. Similar cluster properties under time translations are proven in J. R. Taylor, "Timelike cluster properties in nonrelativistic scattering," *J. Mathematical Phys.* **8** (1967), 2131–2137. The study of these properties was motivated by a discussion of cluster properties to be expected for relativistic S operators in E. H. Wichmann and J. H. Crichton, "Cluster decomposition properties of the S-matrix," *Phys. Rev.* **132** (1963), 2788–2799. Cluster properties for the S-matrix derived from a quantum field theory obeying the Wightman axioms and possessing a mass gap are proven in K. Hepp, "Spatial cluster decomposition properties of the S-matrix," *Helv. Phys. Acta* **37** (1964), 659–662 and "One-particle singularities of the S-matrix in quantum field theory," *J. Mathematical Phys.* **6** (1965), 1762–1767. One important consequence of the cluster properties is that a complete knowledge of the scattering states of charge zero determines the scattering of charged particles. For example, one could study electron–electron scattering by considering states with two electrons and two positrons far away. As the positrons are taken to infinity, the cluster property tells us that the electron–electron scattering amplitude will be recovered in the limit.

The Kato–Birman theory has been applied to prove completeness of n-body scattering in the energy range where the system cannot break up into three or more clusters. This result is due to J. M. Combes, "Time dependent approach to nonrelativistic multichannel scattering," *Nuovo Cimento A* **64** (1969), 111–144; see also B. Simon, "Geometric methods in multiparticle quantum systems," *Comm. Math. Phys.* **55** (1977), 259–274, and "N-Body scattering in the two-cluster region," *Comm. Math. Phys.* **58** (1978), 205–210.

References for further study of analytic properties of the scattering amplitude in the two-body case appear in the Notes to Section 7. Analytic properties in the N-body case are partially treated in the work of Faddeev and Hepp quoted above and more fully in P. Federbush, "Results on the analyticity of many-body scattering amplitudes in perturbation theory," *J. Mathematical Phys.* **8** (1967), 2415–2419; M. Rubin, R. Sugar, and G. Tiktopolous, "Dispersion relations for 3 particle scattering amplitudes, I, II," *Phys. Rev.* **146** (1966), 1130–1149; **159** (1967), 1348–1362; and F. Riahi, "On the analyticity properties of the N-body scattering amplitude in non-relativistic quantum mechanics," *Helv. Phys. Acta* **42** (1969), 299–329.

There is a large physics literature on various fascinating aspects of n-body quantum scattering beyond existence and completeness. As an introduction to this literature, the reader should consult the book of Newton quoted in the notes to Section 2, and the books by M. L. Goldberger and K. Watson, *Collision Theory*, Wiley, New York, 1964; and J. Nuttall and K. Watson, *Topics in Several Particle Dynamics*, Holden-Day, San Francisco, 1967.

Section XI.6 The technical details in the proof of Theorem XI.41 can be found in the monograph by B. Simon, *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms*, Princeton Univ. Press, Princeton, New Jersey, 1971. The proof appears primarily in Section IV.5 of the monograph although for Lemma 1, Section II.9 is needed; for Lemma 2, Section III.4 is needed; for Lemma 5, Section V.3 is needed; and Lemma 6 is found in Section V.4. The details for Theorem XI.42 can be found in Section V.5 of the monograph. For the theorem on zeros of a function analytic in the open upper half-plane, continuous in its closure, the reader should consult K. Hoffman, *Banach Spaces of Analytic Functions*, Prentice Hall, Englewood Cliffs, New Jersey, 1962.

Continuum eigenfunction expansions of the type discussed in Theorem XI.41 were first developed for ordinary differential equations in the 1940s by K. Kodaira and E. Titchmarsh, though the general idea of eigenfunction expansions goes back to the work of D. Bernoulli and J. Fourier. For a historical sketch and many references, see Dunford–Schwartz, Vol. II, p. 1581. This ordinary differential equation theory is applicable to Schrödinger operators on $\mathbb{R}^3$ with centrally symmetric potentials since such operators are direct sums of ordinary differential operators (see the appendix to Section X.1). This point of view and the resulting eigenfunction expansions have been developed by T. Green and O. Lanford III, "Rigorous derivation of the phase shift formula for the Hilbert space scattering operator of a single particle," *J. Mathematical Phys.* **1** (1960), 131–140; and J. Weidmann, "Zur Spektral theorie von Sturm–Liouville Operatoren," *Math. Z.* **98** (1967), 268–302. See Appendix 3 to Section 8.

The earliest treatment of continuum eigenfunction expansions associated with partial differential operators is due to A. Ya. Povzner: "On the expansion of arbitrary functions in terms of the eigenfunctions of the operator $-\Delta u + cu$," *Mat. Sb.* **32** (1953), 109–156 (*Amer. Math. Soc. Trans.*, 2nd Series, **60** (1967)). The connection with scattering theory was first emphasized in A. Ya. Povzner, "On Eigenfunction expansions in terms of scattering solutions," *Dokl. Akad. Nauk SSSR* **104** (1955), and T. Ikebe, "Eigenfunction expansions associated with the Schrödinger operators and their application to scattering theory," *Arch. Rational Mech. Anal.* **5** (1960), 1–34. (Erratum: "Remarks on the orthogonality of eigenfunctions for the Schrödinger operator on $\mathbb{R}^n$," *J. Fac. Sci.*, Tokyo Univ., Sect. I, **17** (1970), 355–361.) Povzner required his potentials to have compact support.

The main idea of our proof of Theorem XI.41, namely, that the connection between the Green's function and the eigenfunctions leads via Stone's formula to (82e′), is taken from Ikebe. Ikebe's treatment differs from ours primarily in two related ways. First, he has different conditions on V: He requires only $V(r) = O(r^{-2-\epsilon})$ rather than $V \in L^1$, but his potentials must be Hölder continuous away from a finite set. Secondly, he introduces an auxiliary Banach space to contain the (unmodified) Lippmann–Schwinger function, $\varphi(x, k)$. To solve the Lippmann–Schwinger equation, he has to rely on compact operator theory in arbitrary Banach spaces, and equicontinuity arguments replace the Hilbert–Schmidt criterion in studying the kernel. The trick of factoring the potential $V = |V|^{1/2}V^{1/2}$ and using a modified Lippmann–Schwinger equation is due (independently) to H. Rollnik, "Streumaxima und gebundene Zustande," *Z. Phys.* **145** (1956), 639–653; A. Grossman and T. T. Wu (see the notes to Section 7) and J. Schwartz, "Some non-self-adjoint operators," *Comm. Pure Appl. Math.* **13** (1960), 609–639. By factoring $V = |V|^a V^{1-a}$ with $\frac{1}{4} < a < \frac{3}{4}$, one obtains a modified Lippmann–Schwinger equation with kernel that is Hilbert–Schmidt if $\int |V(x)|^{2a} |V(y)|^{2-2a} |x-y|^{-2}\, dx\, dy < \infty$ and an inhomogeneous term which is L^2 if $\int |V(x)|^{2a}\, dx < \infty$. By Sobolev's inequality, these integrals are finite if $V \in L^{3/2}$. In this way the methods of this section can be used to treat potentials that are $O(r^{-2-\epsilon})$ at ∞ (Problem 57).

Ikebe's method has been used to study Schrödinger operators in $n \neq 3$ dimensions by D. Thoe in "Eigenfunction expansions associated with Schrödinger operators in $\mathbb{R}_n$, $n \geq 4$," *Arch. Rational Mech. Anal.* **26** (1967), 335–356; and for nonlocal potentials by M. Bertero, G. Talenti, and G. A. Viano in "Eigenfunction expansions associated with Schrödinger two-particle operators," *Nuovo Cimento A* **62** (1969), 27–87. A development similar to Ikebe and Thoe but under different conditions may be found in P. Alsholm and G. Schmidt, "Spectral and scattering theory for Schrödinger operators," *Arch. Rational Mech. Anal.* **40** (1971), 281–311.

The Povzner–Ikebe eigenfunction expansion which we discuss in this section should be distinguished from the eigenfunction expansion of Gårding and Gel'fand discussed in K. Maurin, *General Eigenfunction Expansions and Unitary Representations of Topological Groups*, Polish Scientific, Warsaw, 1968. The latter type of expansion is of an abstract type associated with any operator. Its mere existence contains no spectral information; and, in fact, it consists of little more than a convenient form of the spectral theorem. On the other hand, the Povzner–Ikebe expansions contain connections with scattering theory, asymptotic completeness, and the absence of singular continuous spectrum.

Generalizations of the Povzner–Ikebe expansion to a more abstract setting, including some other elliptic differential operators, have been discussed by S. Kuroda in a series of papers: "Stationary theory of scattering and eigenfunction expansions I, II," *Sûgaku* **18** (1966), 74–85, 135–144; "Perturbation of eigenfunction expansions," *Proc. Nat. Acad. Sci. U.S.A.* **57** (1967), 1213–1217; and (the main article in the series) "An abstract stationary approach to perturbation of continuous spectra and scattering theory," *J. Analyse Math.* **20** (1967), 57–117. Kuroda's ideas and methods are closely connected with the "stationary methods" of Friedrichs which we discuss presently and with the methods of Agmon, Kuroda, and Lavine which we treat in Section XIII.8. Notice once again the element of arbitrariness in a division between "scattering theory" and "spectral properties." This work is a precursor to the abstract Kato–Kuroda theory which we discuss at the end of the notes to this section.

Our discussion of the history of eigenfunction expansions would not be complete without some reference to the general context of "stationary methods." In many ways, the "old-fashioned" naïve scattering theory which we describe later in the notes to this section is a stationary picture, but the "modern" stationary version in the physics literature is generally dated back to two important papers: B. A. Lippmann and J. Schwinger, "Variational principles for scattering processes, I," *Phys. Rev.* **79** (1950), 469–480; and M. Gell'Mann and M. L. Goldberger, "The formal theory of scattering," *Phys. Rev.* **91** (1953), 398–408. The Lippmann–Schwinger equation appeared in the first of these. The Gell'Mann–Goldberger paper suggested the use of "abelian limits," that is, the $\lim_{\epsilon \downarrow 0} \int_0^\infty e^{-\epsilon t} f'(t)\, dt$ in place of $\lim_{t\to\infty} f(t)$ (the discrete version of this limit goes back to Abel) and also contained the formula $S = 1 - 2\pi i\, \delta(E - E')T(k, k')$. These stationary methods, that is, methods which do not directly refer to a limit in *time*, have so dominated the physics literature during the past 25 years that the more natural time-dependent view of scattering is often lost! An example where the abelian limit for the wave operators exists and is unitary, even though the ordinary wave operators do not exist, can be found in J. Howland, "Banach space techniques in the perturbation theory of self-adjoint operators with continuous spectrum," *J. Math. Anal. Appl.* **20** (1967), 22–47.

T. Ikebe, in "On the phase shift formula for the scattering operator," *Pacific J. Math.* **15** (1965), 511–523, proved Theorem XI.42 for the class of potentials obeying his form of the eigenfunction expansion.

There is a second set of ideas going under the name "stationary methods" in the mathematical literature. The method and extensive references are discussed in Section X.5 of Kato's book (referred to in the notes to Section 3). Many of the ideas in the method go back to Friedrichs' 1948 paper (see the notes to Section 3). The basic equation in the theory is an integral equation which is used in the proof of the Kato–Birman theorem appearing in Kato's book. For simplicity, suppose H_0 and V are bounded, $H = H_0 + V$, and that H_0 has purely absolutely continuous spectrum. Then, if $\Omega^-(H, H_0)$ exists

$$\Omega^- = 1 + i\int_0^\infty e^{itH_0} V\Omega^- e^{-itH_0}\, dt$$

If one introduces the symbol, Γ^+ for the operation $T \mapsto \Gamma^+(T) = i\int_0^\infty e^{itH_0} T e^{-itH_0}\, dt$ when the integral exists (converging in the strong topology), then one finds the **Friedrichs' equation**

$$\Omega^- = 1 + \Gamma^+(V\Omega^-) \tag{338}$$

The point is that $\Gamma^+(T)$ has two abstract properties: (a) $T = \Gamma^+(T)H_0 - H_0\Gamma^+(T)$; (b) $\Gamma^+(T)e^{itH_0} \to 0$ strongly as $t \to \infty$. Thus $\Gamma^+(\cdot)$ can be thought of as an "inverse" of $[H_0, \cdot]$ obeying the "boundary condition" (b). The abstract properties (a) and (b) completely characterize $\Gamma^+(T)$. Using this characterization of Γ^+, it is sometimes possible to solve (338) by iteration, at least if V is "small" in some sense. Once again, there is a connection with spectral analysis. We discuss a closely connected technique in Section XIII.7.

Theorem XI.43a appeared in C. Zemach and A. Klein, "The Born expansion in non-relativistic quantum theory, I," *Nuovo Cimento* **10** (1958), 1078–1087. The extension to n dimensions is discussed in W. Faris, "Perturbations of non-normalizable eigenvectors," *Helv. Phys. Acta* **44** (1971), 930–936, and "Time decay and the Born series," *Rocky Mountain J. Math.* **1** (1971), 637–648. Theorem XI.43b is due to M. Scadron, S. Weinberg, and J. Wright, "Functional analysis and scattering theory," *Phys. Rev.* **135** (1964), B202–B207. Related results on small coupling constant scattering theory are discussed in Sections XIII.7, XII.8, and their notes. The use of summability methods, and in particular of Padé approximants, to "sum" the Born series in regions where it diverges is discussed in J. R. Chisholm, "Solution of linear integral equations using Padé approximants and the Jost function," *Nuovo Cimento A* **61** (1969), 747–754, and J. L. Basdevant and B. W. Lee, "Padé approximation and bound states: Exponential potential," *Nuclear Phys. B* **13** (1969), 182–188.

Now, we would like to discuss the "naïve scattering theory" which goes back to M. Born, "Quantenmechanik der Stossvorgänge," *Z. Phys.* **38** (1926), 803–827. This is intended to put Theorem XI.41 in perspective and to provide a link with what the reader may have seen in quantum mechanics textbooks. In a typical scattering experiment, a beam of *nearly* constant energy E is sent into a target. Suppose that the target contains N particles. In the usual approximation, one supposes that the result is N times the scattering from a single target particle. This approximation depends on several factors which are valid in most experiments (when they are not valid, a more complicated analysis is needed): (1) The target particles are much farther apart than the "range" of the forces, that is, the characteristic falloff of the forces. The typical separation of particles in a solid target is $R_0 \cong 10^{-8}$ cm, and typical forces in nuclear experiments have a range $\cong 10^{-13}$ cm. (2) It must be a good approximation that a beam particle does not scatter off more than one target particle in going through the target. If we picture the target as being made of "sheets" 10^{-8} cm apart, the probability of scattering in any sheet is about $\sigma/\pi R^2$ where σ is the total cross section and R is the separation in the target. Since $\sigma < 10^{-25}$ cm^2 for typical nuclear experiments, this probability $\cong 10^{-9}$. Thus in a target with a thickness of 10^{-2} cm, the "probability" of a multiple collision is about 10^{-3}, so this second approximation is "typically" valid. (3) According to the picture of quantum mechanics, we cannot think of a given beam particle as scattering off a particular target particle. Rather, there are amplitudes for scattering off each target particle, and the observed amplitude is the square of the N individual amplitudes. For this to be about N times the square of a typical amplitude, we need to know that there is no interference effect. This requires the deBroglie wavelength of the beam particles λ_D to be much smaller than the interparticle separation. Again, in a nuclear experiment, if incident protons have an energy of 10 MeV, $\lambda_0 \cong 10^{-13}$, which is much smaller than R. Thus, in a typical situation, we can suppose the beam is scattering off a single target particle if we remember the right multiplicative factors involving the number densities of the target and the incident beam.

The next approximation is to suppose that the beam is "infinite" in extent. While mathematically this is somewhat severe since it leads to nonnormalized states, physically it is much milder than the approximations (1)–(3) above! Thus we picture a plane wave e^{ikz} as "input." This wave has momentum $\langle 0, 0, k\rangle$ in $\mathbb{R}^3$ (in units with $\hbar = 1$), so it represents a plane wave "entering" from $z = -\infty$. After the scattering, if we look very far from the target, we expect an outgoing wave, moving out in a spherical pattern but with an angular dependent density. If V is spherically symmetric, then for large r it should have the form $f(\theta)e^{ikr}/r$ where $f(\theta)$ is a quantity which describes the scattering. The $+$ in e^{+ikr}, which we shall see is connected with the sign in the Lippmann-Schwinger equation, is necessary for the wave to be *outgoing*, that is, for the momentum to point outward. The input beam density per unit area/per unit time is $1/v$ where v is the velocity in the particle. If we look at an area of size $r^2\, d\Omega$ about an angle θ, we observe $\{[|f(\theta)|^2/r^2]r^2\, d\Omega\}/v$ particles per unit time. Thus the differential cross section is given by

$$d\sigma/d\Omega = |f(\theta)|^2$$

The basic ansatz of naïve scattering theory is that the "scattering state" is an eigenfunction of the Schrödinger equation which has the asymptotic form $e^{ikz} + f(\theta)e^{ikr}/r$ *for large* r. On the surface, this ansatz looks absurd, for, if $\varphi \sim_{r\to\infty} e^{ikz} + f(\theta)r^{-1}e^{ikr}$, then *at all times* φ has both a plane wave coming in and an outgoing spherical wave. Of course we cannot expect to do better with a stationary picture! Moreover, if we consider a state which at time 0 is $\int g(k)\varphi(x, k)\, dk$, then for large r *and* t it will have the form $\int g(k)e^{ik(z-kt)}\, dk + f(\theta)r^{-1}\int g(k)e^{ik(r-kt)}\, dk$. Then, essentially by the Riemann-Lebesgue lemma, the first integral for z and t large and g peaked near k_0 has appreciable size only if $z \cong k_0 t$ and the second integral if $r \cong k_0 t$. We thus see that if $t \to -\infty$, the second integral is negligible for all r (since $r \geq 0$). Thus, we can expect to recover a time-dependent picture by forming "packets" of the naïve-type wave functions. In fact, this picture can be directly justified. See the third appendix to Section 8.

We remark that some attempts at justifying $d\sigma/d\Omega = |f(\theta)|^2$ starting from the rigorous definition of the S-operator are to be found in J. Dollard, "Scattering into cones, I: Potential scattering," *Comm. Math. Phys.* **12** (1969), 193–203; and J. Jauch, R. Lavine, and R. G. Newton, "Scattering into cones," *Helv. Phys. Acta* **45** (1972), 325–330.

The naive scattering theory method can be summarized as seeking functions $\varphi(x, k)$ that "obey" $H\varphi = k^2\varphi$ and $\varphi(x, k) \sim_{|x|\to\infty} e^{ikz} + f(\theta)r^{-1}e^{ikr}$. $f(\theta)$ is then interpreted as a function whose square gives the differential cross section. Let us present a formal derivation to show that $\varphi(x, k)$ should obey the Lippmann-Schwinger equation. Write $\varphi = e^{ikz} + \eta$. Then $(H - k^2)\varphi = 0$ implies that $(H_0 - k^2)\varphi = -V\varphi$ or $(H_0 - k^2)\eta = -V\varphi$. Thus formally $\eta = -(H_0 - k^2)^{-1}V\varphi$ or φ obeys $\varphi = e^{ikz} - (H_0 - k^2)^{-1}V\varphi$. Of course, the inverse $(H_0 - k^2)^{-1}$ is not well defined. As we shall presently see, the choice $\varphi = e^{ikz} - [H_0 - (k^2 + i0)]^{-1}V\varphi$ is directly connected with the desire that for large r, $\varphi - e^{ikz} \sim e^{ikr}r^{-1}f(\theta)$ and not $e^{-ikr}r^{-1}f(\theta)$.

We thus identify the naïve wave function φ with the Lippmann-Schwinger function. Therefore, φ obeys (with $\mathbf{k} = \langle 0, 0, k\rangle$)

$$\varphi(\mathbf{x}, k) = e^{ikz} - (4\pi)^{-1}\int e^{ik|\mathbf{x}-\mathbf{y}|}|\mathbf{x} - \mathbf{y}|^{-1}V(\mathbf{y})\varphi(\mathbf{y}, \mathbf{k})\, d\mathbf{y}$$

For $|\mathbf{x}|$ large, $|\mathbf{x} - \mathbf{y}|^{-1} \cong |\mathbf{x}|^{-1}$ and $\exp(ik|\mathbf{x} - \mathbf{y}|) \cong \exp(ik|\mathbf{x}| - ik\cdot\hat{\mathbf{x}}|y|) = \exp(ik|\mathbf{x}| - ik|\mathbf{y}|\cos\theta)$ where θ is the angle between x and y. Thus, formally,

$$\varphi(\mathbf{x}, \mathbf{k}) \underset{|\mathbf{x}|\to\infty}{\sim} e^{i\mathbf{k}\cdot\mathbf{x}} + |\mathbf{x}|^{-1}e^{ik|\mathbf{x}|}f(\theta)$$

where

$$f(\theta) = -(4\pi)^{-1}\int e^{-i\mathbf{k}'\cdot\mathbf{y}}V(\mathbf{y})\varphi(\mathbf{y}, \mathbf{k})\, d\mathbf{y} = -2\pi^2 T(\mathbf{k}', \mathbf{k})$$

if $\mathbf{k}'$ is defined by $k' = k$ and $\mathbf{k}\cdot\mathbf{k}' = \cos\theta$. The above argument represents a formal justification of (96) and (97a).

Note that if we took φ to obey $\varphi = e^{ikz} - [H_0 - (k^2 - i0)]^{-1}V\varphi$, the above analysis would have led to $\varphi \sim_{r\to\infty} e^{ikz} + \tilde{f}(\theta)r^{-1}e^{-ikr}$. Our desire to have $\varphi - e^{ikz} \sim e^{+ikr}r^{-1}$ for large $|x|$ is thus directly connected with the "$+i0$ prescription" in the Lippmann-Schwinger equation.

The abstract approach to eigenfunction expansions is intimately related to the results of Section XIII.8 where the reader can find extensive references including a history. Here we note that a systematic theory has been developed by T. Kato and S. Kuroda, "Theory of simple scattering and eigenfunction expansions," in *Functional Analysis and Related Fields*, pp. 99–131, Springer-Verlag, New York, Heidelberg, Berlin, 1970. Applications of these ideas to multiparticle scattering can be found in the Howland reference in the notes to Section 5.

It is well known that the resolvent can be analytically continued in a suitable sense when the potential falls off exponentially. See, for example, the second Grossman-Wu paper quoted in the notes to Section 7, Simon's monograph quoted above, C. Dolph, J. McLeod, and D. Thoe, "The analytic continuation to the unphysical sheet of the resolvent kernal and the scattering operator associated to the Schrödinger operator," *J. Math. Anal. Appl.* **16** (1966), 311–332, or the series of papers by N. Shenk and D. Thoe, "Eigenfunction expansions and scattering theory for perturbations of $-\Delta$," *J. Math. Anal. Appl.* **36** (1971), 313–351; *Rocky Mountain J. Math.* **1** (1971), 89–125.

Section XI.7 The original motivation for study of the analytic properties of the scattering amplitude came from outside the realm of potential scattering theory. The earliest dispersion relations were proven for the index of refraction in an optical medium by R. Kronig, "On the theory of dispersion of x-rays," *J. Amer. Optical Soc.* **12** (1926), 547–558, and by H. A. Kramers, Atti del Congress Int. de Fisica, Como (1927).

In the early 1950s "dispersion theory" developed as a method of analyzing and interpreting scattering data in elementary particle physics. The progression of the development of any aspect of the theory was typically in four stages: First, a suggestion of some analyticity property was made. Next, someone found a "proof" of the property which was far from rigorous but which emphasized the physical reasons why the property should be true. Third, a rigorous proof was found in a quantum field theory framework—such rigorous proofs did not start from the Wightman axioms but from the stronger L.S.Z. framework. (Only much later was the L.S.Z. framework derived from the Wightman axioms together with additional assumptions; see Section 16 and its notes.) Finally, using some ideas from the field theory proof, a proof of the analogous property in potential scattering was developed. In some cases, stage three was never completed although stage four was successful.

The early history of dispersion theory is quite complicated and is summarized in Chapter 10 of the book of Goldberger and Watson quoted in the notes to Section 5. We note the three fundamental papers: R. Kronig, "A supplementary condition in Heisenberg's theory of elementary particles," *Physica* **12** (1946), 543–544; M. Gell'Mann, M. L. Goldberger, and W. Thirring, "Use of causality conditions in quantum theory," *Phys. Rev.* **95** (1954), 1612–1627; and M. L. Goldberger, "Use of causality conditions in quantum theory," *Phys. Rev.* **97** (1955), 508–510. This last paper contained a heuristic "derivation" of forward dispersion relations for pion-nucleon scattering. The first rigorous proof in a field theory (L.S.Z.) framework is due to K. Symanzik, "Derivation of dispersion relations for forward scattering," *Phys. Rev.* **105** (1957),

743–749. The earliest proof of a potential scattering forward dispersion relation (a weak version of Theorem XI.46) is due to N. Khuri, "Analyticity of the Schrödinger scattering amplitude and non-relativistic dispersion relations," *Phys. Rev.* **107** (1957), 1148–1156. Khuri used a Fredholm theory formulation of potential scattering due to R. Jost and A. Pais, "On the scattering of a particle by a static potential, *Phys. Rev.* **82** (1951), 840–851. Theorem XI.46 with a proof closely related to the one we give is due to A. Grossman and T. T. Wu, "Schrödinger scattering amplitude, I," *J. Mathematical Phys.* **3** (1961), 710–713.

Nonforward dispersion relations, that is, the analyticity of $f(\cdot, \Delta)$ for fixed real Δ, were first suggested by five groups of physicists approximately simultaneously: by Goldberger, Nambu and Oehme (unpublished), by Gell'Mann and Polkinghorne (unpublished), by Symanzik (unpublished), by A. Salam, "On generalized dispersion relations," *Nuovo Cimento* **3** (1956), 424–429, and by R. Capps and G. Takeda, "Dispersion relations for finite momentum-transfer pion–nuclear scattering," *Phys. Rev.* **103** (1956), 1877–1896. Rigorous field theory proofs are due to N. N. Bogoliubov, B. V. Madvedev, and M. K. Polivanov, "Probleme der Theorie der Dispersionsbeziehungen," *Fortschr. Physik* **6** (1958), 169–246; and H. Bremmerman, R. Oehme, and J. G. Taylor, "Proof of dispersion relations in quantized field theories," *Phys. Rev.* **109** (1958), 2178–2190. Discussion of analyticity in Δ for fixed k is due to H. Lehmann, "Scattering matrix and field operators," *Nuovo Cimento Suppl.* **14** (1959), 153–176. In potential scattering, the earliest version of Theorem XI.47 is due to W. Hunziker, "Regularitätseigenschaften der Streuamplitude im Fall der Potentialstreuung," *Helv. Phys. Acta* **34** (1961), 593–620. A proof using the factorization of the potential appears in A. Grossman and T. T. Wu, "Schrödinger scattering amplitude, III," *J. Mathematical Phys.* **3** (1962), 684–689.

A proof of Theorem XI.47 may be found in Chapter 6 of Simon's monograph quoted in the notes to Section 6. The only theorem explicitly stated there involves analyticity in D_α, but the proof works for any D_β with $0 < \beta \leq \alpha$.

Generalized Yukawa potentials, often under the name Yukawian potentials, have been extensively studied because they are believed to be the closest nonrelativistic analogues of the situation in relativistic scattering. A summary of the various analyticity results for such potentials including a proof of Theorem XI.48 can be found in the book by V. De Alfaro and T. Regge, *Potential Scattering*, North Holland, Amsterdam, 1965. The most interesting results for Yukawian potentials involve joint analyticity in Δ and E and the related Mandelstam representation—see Section V.6 and its notes for a discussion of this theory.

In addition to the analyticity results discussed in this section there are three other broad classes of analyticity results. First, there are some analyticity results for N-body scattering—references for this may be found in the notes to Section 5. Secondly, there are results on the analyticity of individual partial wave amplitudes—these are discussed in Section 8. Finally, there are the results on analyticity in angular momentum which we briefly discuss in the notes to Section 8.

As we explained in Section 1, the physical intuition behind analyticity depends on causality. This connection is well disguised in the proofs of this section for the following reason: The causality intuition is time dependent, while our proofs used time-independent methods. The Lax–Phillips theory of Section 11 is a time-dependent framework for scattering theory based directly on causality. As a result, the analyticity properties arise naturally from the causality in the Lax–Phillips approach. However, because of technical difficulties, the Lax–Phillips theory applies to scattering in nonrelativistic quantum mechanics only for a very restricted class of potentials.

Section XI.8 References to articles which describe the theory of eigenfunction expansions for central potentials can be found in the Notes to Section 6. The development of much of the spectral analysis of Chapter XIII for this special class of potentials appears in J. Weidmann, "Zur Spektraltheorie von Sturm–Liouville Operatoren," *Math. Z.* **98** (1967), 268–302.

It is no coincidence that the scattering amplitude as found in Theorem XI.53 automatically obeys unitarity. There is a general principle that implies that when H and H_0 both have simple spectra (and this is true on each subspace of fixed angular momentum) $\Omega^\pm(H, H_0)$ exist, $\sigma_{ac}(H) \subset \sigma_{ac}(H_0)$, and the absolutely continuous spectrum for H_0 obeys a technical condition, then $\Omega^\pm(H, H_0)$ are complete. This result is discussed in Problems 87 and 88. The basic idea appears in Kuroda's *Nuovo Cimento* paper quoted in the Notes to Section 4. An error in his paper is corrected in the paper of Deift and Simon quoted in the Notes to the same section.

Theorems of the genre of Theorem XI.49 are behind Kuroda's theory of eigenfunction expansions (see the Notes to Section XI.6 and XIII.8); see especially T. Kato and S. Kuroda, "The abstract theory of scattering," *Rocky Mountain J. Math.* **1** (1971), 127–171. Our development follows closely that of T. Kato in "Scattering theory," pp. 90–113 in *Studies in Applied Math.* (A. H. Taub, ed.), Math. Assoc. Amer., Buffalo, New York, 1971. S. Kuroda, in "Scattering theory for differential operators, I," *J. Math. Soc. Japan* **25** (1973), 75–104, has shown that the fibers $T(E)$ are in certain $\mathscr{S}_p$ classes depending on the precise falloff of V. He allows slower falloff than we discuss in Theorem XI.49.

The basic connection between time delay and the phase of the quantum scattering amplitude is a discovery of L. Eisenbud, Ph.D. Thesis, Princeton Univ. 1948 (unpublished); see E. P. Wigner, "Laws/limit for the energy derivative of the scattering phase shift," *Phys. Rev.* **98** (1955), 145–147. Further discussion can be found in J. M. Jauch and J. P. Marchand, "The time delay operator for simple scattering systems," *Helv. Phys. Acta* **40** (1967), 217–229; and J. M. Jauch, K. B. Sinha, and B. N. Misra, "Time-delay in scattering processes," *Helv. Phys. Acta* **45** (1972), 398–426.

Compactness of $S(E) - I$ in certain three-body systems has been proven by R. Newton, "The three particle S-matrix," *J. Mathematical Phys.* **15** (1974), 338–343.

Like so much else, the partial wave expansion and the connection to eigenfunctions (Theorem XI.53) go back to the classic *Theory of Sound*, 2nd ed. of Lord J. W. S. Rayleigh, Macmillan, London, 1894. The use of partial wave expansions in quantum scattering was first suggested by M. Faxen and J. Holtsmark, "Beitrag zur Theorie des Durchganges langsamer Elektronen durch Gase," *Z. Phys.* **45** (1927), 307–324.

That the natural domain of convergence of Legendre series is an ellipse is a discovery of K. Neumann, *Über die Entwickelung einer Funktion mit imaginärem Argument, nach der Kugelfunktionen erster und zweiter Art*, Halla, Verlag Von Schmidt 1862; and L. W. Thome, "Über die Reihen welche Nach Kugelfunktion fortschreiten," *J. Math.* **66** (1866), 337–343. Earlier, E. Heine, "Theorie der Anziehung eines Ellipsoids," *J. Math.* **42** (1851), 70–82, had proven the basic (137). There is a long discussion of Legendre series based on the analogy with Taylor series in T. Kinoshita, J. J. Loeffel, and A. Martin, "Upper bounds for the scattering amplitude at high energy," *Phys. Rev. B* **135** (1964), 1464–1482.

The connection between ordinary differential equations and integral equations via the method of variation of parameters is a standard feature of the theory of ordinary differential equations. The closest analogue for partial differential equations is the method of Green's functions. An important difference between the situation for ordinary differential equations and that for partial differential equations is that the integral equation in the former case is a **Volterra equation** $f(x) = g(x) + \lambda \int k(x, y) f(y)\, dy$ where $k = 0$ if $x \leq y$. Such equations have the property that their Neumann series $I + \lambda K + \lambda^2 K^2 + \cdots$ is convergent for all λ; in more modern terminology the operator is quasi-nilpotent, that is, $\sigma(K) = \{0\}$. It is for this reason that the possibility of an exceptional set $\mathscr{E}$ occurs in the study of the Lippmann–Schwinger equation, which corresponds

to the partial differential equation—$\Delta\varphi + V\varphi = E\varphi$, but not in the study of the regular and Jost equations, which correspond to the ordinary differential equation $-u'' + Vu = Eu$.

The variable phase equation approach including extensive developments is due to F. Calegero; see especially his book, *The Variable Phase Approach to Potential Scattering*, Academic Press, New York, 1967. There is a connection between Theorems XI.55, XI.59, and the assertion of Theorem XIII.8 that $n_\ell(V)$ is the number of zeros of $u_\ell(r; E)$—any two imply the third. Notice that our proofs of these results use quite different methods. In particular, one can prove Levinson's theorem without recourse to analytic properties of the Jost function or the construction of Jost solutions.

A thorough discussion of partial wave amplitudes, Jost functions, etc. including the $\ell > 0$ case can be found in the monograph of V. de Alfaro and T. Regge quoted in the Notes to Section 7.

The Jost function formalism for s-wave scattering was presented in R. Jost, "Über die falschen Nullstellen der Eigenwerte der S-Matrix," *Helv. Phys. Acta* **20** (1947), 250–266; and further developed in V. Bargmann, "On the connection between phase shifts and the scattering potential," *Rev. Modern Phys.* **21** (1949), 488–493. Jost's original definition was that $\eta(k) \equiv \eta(0, k)$. The definition as a Wronskian is a later refinement especially useful for $\ell > 0$ where $x = 0$ is a singular point. The symbols $\eta(x, k)$, $\eta(k)$ are not standard; $f(x, k)$ and $f(k)$ are more usual—but since f is also used for the scattering amplitude, we have decided to use η. As we describe in the Notes to Section XIII.17, the Jost function is a (Fredholm) determinant associated with the radial Lippmann-Schwinger equation.

The behavior of $\eta(k)$ for the potential λV as a function of the coupling constant λ, especially as $\lambda \to \infty$, has been studied by K. Chadan, "The asymptotic behavior of the number of bound states of a given potential in the limit of large coupling," *Nuovo Cimento* **58** (1968), 191–204; and W. M. Frank, "Strong coupling limit in potential theory I, II," *J. Mathematical Phys.* **8** (1967), 466–476; **9** (1968), 1890–1898. Of particular interest is the connection between this behavior and the number of spherically symmetric bound states $n(\lambda V)$ of $-\Delta + \lambda V$. It is proven for a wide class of potentials that $\lim_{\lambda\to\infty} n(\lambda V)/\lambda^{1/2} = \pi^{-1} \int |V_-(x)|^{1/2}\, dx$ where $V_- = \max\{-V, 0\}$. We shall prove this by very different means in Section XIII.15.

Levinson's theorem was proven in N. Levinson, "On the uniqueness of the potential in a Schrödinger equation for a given asymptotic phase," *Danske Vid. Selsk. Mat.-Fys. Medd.* **25** (1949). For partial waves with $\ell > 0$, a detailed discussion of Levinson's theorem especially when $f(0) = 0$ (and Jost function theory in general) may be found in R. G. Newton, "Analytic properties of radial wave functions," *J. Mathematical Phys.* **1** (1960), 319–347.

The proof of Theorem XI.61 by a method similar to the one we use appears in A. Bottino, A. M. Longoni, and T. Regge, "Potential scattering for complex energy and angular momentum," *Nuovo Cimento* **23** (1962), 954–1004. A similar result, proven by a different method, appears in L. Brown, D. Fivel, B. W. Lee, and R. F. Sawyer, "Fredholm method in potential scattering and its application to complex angular momentum," *Ann. Physics* **25** (1963), 187–220.

For generalized Yukawa potentials, the discontinuities of $f_0(k^2)$ across the cut $(-\infty, -\mu_0^2)$ can be computed directly from the weight C in $\int_{\mu_0}^{\infty} C(\mu)e^{-\mu x}\, d\mu$; by an iterative procedure, one obtains the discontinuity in the interval $[-(n+1)^2\mu_0^2, -n^2\mu_0^2]$ at the nth stage. This method was developed in A. Martin, "On the analytic properties of partial wave scattering amplitudes obtained from Schrödinger's equation," *Nuovo Cimento* **14** (1959), 403–425, and "Analytic properties of $\ell \neq 0$ partial wave amplitudes for a given class of potentials," *Nuovo Cimento* **15** (1962), 99–109; it is further discussed in the book of DeAlfaro and Regge.

For generalized Yukawa potentials, the discontinuities across the cuts are especially important because $s_0(k^2)$ is polynomially bounded (in fact it approaches 1 as $k \to \infty$) so that dispersion relations can be written. This is a critical distinction from C_0^∞ potentials where the Jost function is entire (and $f_0(E)$ is meromorphic in $\mathbb{C}\backslash[0, \infty)$). In this case $s_0(k^2)$ does not have polynomial growth as $k \to \infty$.

Variational methods like the Kohn formula (136c) are of interest since they suggest that the error between a and $\beta(\psi) - (h\psi, \psi)$ is only the magnitude of the square of the error between ψ and φ. On this basis methods were developed for general phase shifts by various authors: L. Hulthén, "Variational problem for the continuous spectrum of a Schrödinger equation," *Kgl. Fys. Salla Lund Fortschn.* **14** (1944), 1–13, and W. Kohn, "Variational methods in nuclear collision problems," *Phys. Rev.* **74** (1948), 1763–1772. A third principle is due to J. Schwinger in unpublished lecture notes; the method is described in J. Blatt and J. Jackson, "On the interpretation of neutron-proton scattering data by the Schwinger variational method," *Phys. Rev.* **76** (1949), 18–37. That the principles could lead to rigorous bounds under suitable circumstances was realized by T. Kato in a series of papers, "Variational methods in collision problems," *Phys. Rev.* **80** (1950), 475, "Notes on Schwinger's variational method," *Progr. Theoret. Phys.* **6** (1951), 295–305, and "Upper and lower bounds on scattering phases," *Progr. Theoret. Phys.* **6** (1951), 394–407. The bound we give in Theorem XI.61.5 and its proof are given by L. Spruch and L. Rosenberg, "Upper bounds on scattering lengths for static potentials," *Phys. Rev.* **116** (1959), 1034–1040, and further discussed in their papers: "Upper bounds on scattering lengths for compound systems: n-D quartet scattering," *Phys. Rev.* **117** (1960), 1095–1102; "Bounds on scattering phase shifts: Static central potentials," *Phys. Rev.* **120** (1960), 474–482; "Bounds on scattering phase shifts for compound systems," *Phys. Rev.* **121** (1961), 1720–1726; and "Minimum principle for multi channel scattering," *Phys. Rev.* **125** (1962), 1407–1414. The effect of bound states on the bounds is discussed in L. Rosenberg, L. Spruch, and T. O'Malley, "Upper bounds on scattering lengths when composite bound states exist," *Phys. Rev.* **118** (1960), 184–192. Rosenberg-Spruch note that their bounds also can be proven with the methods Kato used earlier. The reader may have noticed that while (136d) is a lower bound, Rosenberg-Spruch refer to an upper bound. This is because they use the opposite sign convention for a from the one we use. Their convention, which makes the scattering length of a hard sphere positive (and equal to its radius), is slightly more common in the literature than ours, but both conventions are frequently used.

There is a rather large literature on oscillatory potentials. Discussion of scattering for noncentral potentials with severe oscillations at infinity (of the kind occurring in Example 1 of Appendix 2) can be found in V. B. Matveev and M. M. Skriganov, "Wave operators for the Schrödinger equation with rapidly oscillating potential," *Dokl. Akad. Nauk SSSR* **202** (1972), 755–758, M. M. Skriganov, "Spectrum of the Schrödinger operator with strongly oscillating potentials," *Trudy. Stek. Math.* **125** (1973), 183–195; M. Combescure and J. Ginibre, "Spectral and scattering theory for the Schrödinger operator with strongly oscillating potentials," *Ann. Inst. H. Poincaré Sect. A* **24** (1976), 17–29; M. Schechter, "Spectral and scattering theory for elliptic operators of arbitrary order," *Comment. Math. Helv.* **49** (1974), 84–113, and "Scattering theory for the Schrödinger equation with potentials not of short range," Jubilee Volume Dedicated to the 70th Anniversary of Academician I. N. Vekua, USSR Acad. Sci., 1977. In particular, the quadratic form construction outlined in Example 1 is due independently to Combescure, Ginibre, and Schechter. These authors also derive stronger results in the scattering theory for these potentials than appear in the text by using the methods of Section XIII.8.

Because of Pearson's example (see Section 4), there has been discussion of oscillations near zero, see, for example, W. O. Amrein and V. Georgescu, "Strong asymptotic completeness of wave operators for highly singular potentials," *Helv. Phys. Acta* **47** (1974), 517–533; and M. L. Baetman and K. Chadan, "Scattering theory with highly singular oscillating potentials," *Ann. Inst. H. Poincaré Sect. A* **24** (1976), 1–16. These local oscillations can be controlled by the method of Theorem XI.68. In particular, Baetman and Chadan analyze the regular integral

equation with oscillatory potentials in much the same way we analyze the Jost equation in Example 1, revisited. In fact, we have closely followed their approach, concentrating on $r = \infty$ in place of $r = 0$. The absence of positive eigenvalues in this case (Theorem XI.68a) seems to be a new result although it could have been proven by Baetman and Chadan had they considered oscillations at infinity.

Parts (a) and (c) of Theorem XI.67 are due to F. Atkinson, "The asymptotic solutions of second order differential equations," *Ann. Mat. Pura Appl.* **37** (1954), 347–378.

Theorem XI.66 is due to J. Dollard and C. Friedman, "On strong product integration," *J. Functional Analysis* **28** (1978), 309–354. Their application to recover some of Atkinson's results and also Theorem XI.67b appears in their paper, "Product integrals and the Schrödinger equation," *J. Mathematical Phys.* **18** (1977), 1598–1607.

Theorem XI.69 is an abstraction of an argument of T. A. Green and O. E. Lanford, III, "Rigourous derivation of phase shift formula for the Hilbert space scattering operator of a single particle," *J. Mathematical Phys.* **1** (1960), 139–148. These authors also go further to allow potentials in Corollary 1 with $|V(x)| \leq C|x|^{-1-\epsilon}$; they do this by considering higher order contributions in the Jost solution series. The application of the theory in combination with Theorem XI.67 is due to J. Dollard and C. Friedman, "Existence of the Møller wave operators for $r^{-\beta}\lambda \sin(\mu r^{\alpha})$," *Ann. Phys.* **111** (1978), 251–266.

Existence and completeness of the wave operators, but only for sufficiently high energies, for noncentral potentials with behavior like $r^{-1} \sin r$ at infinity has been obtained by K. Mochizuki and J. Uchiyama, 1977 Nagoya Institute of Technology, preprint.

The results of the appendices show how subtle the phenomenon of positive eigenvalues really is. For example, suppose that $V(r) \sim Cr^{-1} \sin(r^{\alpha})$ for large r. If $\alpha < 1$, then $\partial V/\partial r = O(r^{-1-\epsilon})$, so no positive eigenvalues can occur by Theorem XIII.58. If $\alpha > 1$, then $\int_x^\infty V(r)\, dr = O(r^{-1-\epsilon})$, so no positive eigenvalues can occur by Theorem XI.68. It is only for $\alpha = 1$ that such eigenvalues can occur and then they actually do occur sometimes.

We close the notes of this section, our last on short-range nonrelativistic quantum scattering with a brief description of *some* of the topics which we have *not* touched upon in the text or notes:

(1) One of the most interesting is the theory of analytic continuation of the quantities $f_\ell(E)$ in ℓ. This idea is due to T. Regge, "Introduction to complex orbital momenta," *Nuovo Cimento* **14** (1959), 951–976; and is further discussed by R. G. Newton, *The Complex J-Plane: Complex Angular Momentum in Non-Relativistic Quantum Scattering Theory*, Benjamin, New York, 1964. For an introduction to the use of the method in particle physics, see P. D. B. Collins and E. U. Squires, *Regge Poles in Particle Physics*, Springer-Verlag, New York, Heidelberg, Berlin, 1968.

(2) The "inverse problem" of reconstructing the potential given $\delta_\ell(k)$; the basic paper is that of I. M. Gel'fand and R. M. Levitan, "On the determination of a differential equation from its spectral function," *Izv. Akad. Nauk SSSR Ser. Math.* **15** (1951), 309–360; for a more complete history and a discussion of the Gel'fand–Levitan method, see Chapter 12 of the Regge–deAlfaro monograph. For lucid reviews, including more recent work, see Z. S. Agranovich and V. A. Marchenko, *The Inverse Problem of Scattering Theory*, Gordon and Breach, New York, 1963; L. D. Faddeev, "The inverse problem in the quantum theory of scattering," *J. Mathematical Phys.* **4** (1963), 72–104; L. D. Faddeev, "Properties of the S-matrix of the one dimensional Schrödinger equation," *Trudy. Mat. Inst. Steklov* **73** (1964), 314–333 (*Amer. Math. Soc. Transl.* **65**, 139–166) and J. J. Loeffel, "On an inverse problem in potential scattering theory," *Ann. Inst. H. Poincaré Sect. A* **8** (1968), 339–447. A beautiful new approach to the inverse problem can be found in P. Deift and E. Trubowitz, "Inverse scattering on the line," *Comm. Pure Appl. Math.* **32** (1979) (to appear).

(3) The *N/D* method of G. Chew and S. Mandelstam, "Theory of low-energy pion–pion interaction," *Phys. Rev.* **119** (1963), 467–477.

(4) General methods for obtaining information from the analyticity properties of multiparticle scattering amplitudes. This is especially relevant in relativistic scattering theory, but is also of interest in the nonrelativistic theory. For a mathematical discussion, see A. Martin, *Scattering Theory: Unitarity, Analyticity and Crossing*, Lecture Notes in Physics, Number 3, Springer-Verlag, New York, Heidelberg, Berlin, 1969. For discussions emphasizing applications to particle physics and/or the connections with quantum field perturbation theory, see G. Chew, *The Analytic S-Matrix*, Benjamin, New York, 1966; R. J. Eden, *High Energy Collisions of Elementary Particles*, Cambridge Univ. Press, London and New York, 1967; and R. J. Eden, P. V. Landshoff, D. I. Olive, and J. C. Polkinghorne, *The Analytic S-Matrix*, Cambridge Univ. Press, London and New York, 1966.

Section XI.9 Classical Coulomb scattering was first developed by Lord Rutherford as part of his famous experiment which led to the conclusion that atoms had nuclei. Rutherford was very lucky, for the quantum Coulomb cross section just happens to exactly equal the classical one (this miracle is further compounded in that the Born approximation is exact in this case!). Moreover, he was lucky in that the α particles he used were not energetic enough to significantly interact with the nucleus through nuclear forces, so he saw only the Coulomb interaction.

For a discussion of exact solutions of the classical Coulomb problem from a symmetry (Lenz vector) point of view, see H. Abarbanel, "The inverse r-squared force: An introduction to its symmetries," in *Studies in Mathematical Physics, Essays in Honor of Valentine Bargmann* (E. Lieb, B. Simon, A. Wightman, eds.), Princeton Univ. Press, Princeton, New Jersey, 1976.

Long-range classical scattering theory from the point of view we use was developed by I. Herbst, "Classical scattering with long range forces," *Comm. Math. Phys.* **35** (1974), 193–214. All of Theorem XI.73 except for the parts involving (165) are due to Herbst. The discussion of "asymptotically central" potentials is new.

Quantum Coulomb scattering was first treated by W. Gordon, "Über den Stoss zweier Punktladungen nach der Wellenmechanik," *Z. Phys.* **48** (1928), 180–191, who dealt with the eigenfunction expansion for the Coulomb problem working a priori with the time-independent formalism. He found that the continuum eigenfunctions did not look like

$$e^{ik\cdot r} + \frac{e^{ikr}}{r} f(\theta)$$

for r large, but rather like

$$e^{ik\cdot r} + r^{-1} \exp(i[kr + \lambda k^{-1} \ln(4kr)]) f_E(\theta)$$

for r large and $\theta \neq 0$, and identified $f_E(\theta)$ with the Coulomb scattering amplitude. He thus eliminated the infinite phase shifts by fiat.

The time-dependent theory of quantum Coulomb scattering appeared first in J. Dollard, "Asymptotic convergence and the Coulomb interaction," *J. Mathematical Phys.* **5** (1964), 729–738. We use the symbol $U_D(t)$ for this reason. His results were extended to more general long-range potentials by W. O. Amrein, Ph. A. Martin, and B. Misra, "On the asymptotic condition in scattering theory," *Helv. Phys. Acta* **43** (1970), 313–344; V. S. Buslaev and V. B. Matveev, "Wave operators for the Schrödinger equation with a slowly decreasing potential," *Theoret. and Math. Phys.* **2** (1970), 266–274; P. K. Alsholm and T. Kato, "Scattering with long range potentials," in *Partial Differential Equations*, pp. 393–399, Proc. Symp. Pure Math.,

Vol. 23, Amer. Math. Soc., Providence, Rhode Island, 1973; and by L. Hörmander, "The existence of wave operators in scattering theory," *Math. Z.* **146** (1976), 69–91. Amrein et al. extended Dollard's method to allow $r^{-\alpha}$ potentials for $\alpha > \frac{1}{2}$. Buslaev–Matveev and Alsholm–Kato use high order approximate solutions to the Hamilton–Jacobi equation and require information on higher and higher derivatives as the range gets longer and longer; for example, Buslaev–Matveev require $|D^{\alpha}V_L(x)| \leq C(1+x)^{-\varepsilon-|\alpha|}$ for all $|\alpha| \leq k$ where $k = [n/2] + 2 + [1/\varepsilon]$ where $[a] \equiv$ largest integer less than a. The strongest result is due to Hörmander whose paper includes Theorem XI.84. Hörmander dealt with general constant coefficient differential operators for H_0.

Dollard and Hörmander discuss multichannel problems.

Eigenfunction expansions for the purely Coulomb case are discussed in Dollard's paper. Eigenfunctions for general long-range potentials are part of the general subject of spectral analysis of such potentials, and some references can be found in the notes to Section XIII.8. Recent work on the subject includes: T. Ikebe, "Spectral representations for Schrödinger operators with long-range potentials," *J. Functional Analysis* **20** (1975), 158–177; and "Spectral representations for Schrödinger operators with long-range potentials—Perturbation by short-range potentials," *Publ. Res. Inst. Math. Sci.* **11** (1976), 551–558; T. Ikebe and H. Isozaki, "Completeness of modified wave operators for long range potentials," *Pub. RIMS Kyoto* **14** (1978), (to appear); H. Isozaki, "On the long range wave operators," *Publ. Res. Inst. Math. Sci. Pub. RIMS Kyoto* **13** (1977), 589–626; H. Kitada, "Scattering theory for Schrödinger operators with long-range potentials, I, II," *J. Math. Soc. Jap.* **29** (1977), 665–691; G. Pinchuk, "Abstract time independent wave operator theory for long-range potentials," Berkeley thesis, unpublished; Y. Saito, "Eigenfunction expansions for the Schrödinger operator with long-range potentials, $Q(y) = O(|y|^{-\varepsilon})$, $\varepsilon > 0$," *Osaka J. Math.* **14** (1977), 37–53. In addition S. Agmon has announced fairly complete results exploiting extensions of his weighted L^2-space techniques. Finally, V. Enss has informed us that his methods described in Section 17 can be modified to accommodate long range potentials including the Coulomb potential.

The quantum on-energy-shell S-operators for long-range potentials typically are very singular at $k = k'$ (zero scattering angle). In the short-range case, the distribution $s(k, k')$ has only a $\delta(k - k')$ singularity at $k = k'$; in the Coulomb case the singularity is worse; see I. Herbst, "On the connectedness structure of the Coulomb S-matrix," *Comm. Math. Phys.* **35** (1974), 181–191.

Finally, we want to make some remarks about the phase of the Coulomb scattering amplitude. As we have carefully explained, the phase is not determined by the basic time-dependent theory. Nevertheless, there is a sense in which this phase is measurable! To understand this phenomenon we shall have to say something about how dispersion relations are experimentally checked; more information on this of relevance to our discussion can be found in R. Eden, *High Energy Collisions of Elementary Particles*, Cambridge Univ. Press, London and New York, 1967.

One would like to check forward dispersion relations in strongly interacting systems. The problem with doing this is that the only reasonable targets are charged particles, namely the protons in a hydrogen target. Moreover, the easiest projectiles to detect after scattering are charged, say π^+. Since the particles are charged, there are Coulomb forces as well as strong interactions, and an infinite cross section results due to very small angle Coulomb scattering. How does one try to find the "strong part" of the scattering amplitude to check the forward dispersion relations? Physicists make the ansatz:

$$f(\theta) = f_s(\theta) + f_c(\theta) \tag{339}$$

where $f_c(\theta)$ is the "standard" Coulomb amplitude as found by Gordon. We discuss this ansatz further below. Typically, the differential cross section at small angles looks like the solid line in

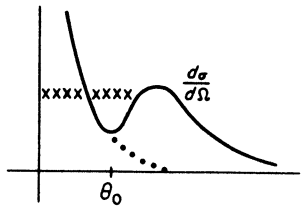


FIGURE XI.18

the schematic Figure XI.18. The dotted line represents the exact value of $|f_c|^2$. How do we "find" $\operatorname{Im} f_s(\theta = 0)$ and $\operatorname{Re} f_s(\theta = 0)$? In the region when f_c is very small, the differential cross section is essentially $|f_s(\theta)|^2$. The crossed line in Figure XI.18 represents an extrapolation of the putative $|f_s(\theta)|^2$ to $\theta = 0$. By integrating this over θ and using the optical theorem, one deduces what $\operatorname{Im} f_s(\theta = 0)$ is. How do we find $\operatorname{Re} f_s(\theta = 0)$? One expects $f_s(\theta)$ to be slowly varying near $\theta = 0$, so we need only find $\operatorname{Re} f_s(\theta = \theta_0)$. The dip at $\theta = \theta_0$ is caused by interference between f_s and f_c at the point where $|f_s| \sim |f_c|$. The magnitude of the dip *and the knowledge of* f_c allow one to find the argument of f_s, and so $\operatorname{Re} f_s(\theta = \theta_0)$. With this, one can check the forward dispersion relations. The point is that if one believes forward dispersion relations, one can turn around the analysis and "measure" the argument of f_c. How does this fit in with the fact that this argument is not determined by the usual time-dependent theory? The key seems to be (339) and the demand of forward dispersion relations. The f_s in (339) will not be the true scattering amplitude for the strong interaction since f is *not* linear in the potential. We thus regard (339) as a definition of f_s. Namely, we *conjecture* the following: With the choice of modified quantum dynamics we made in the Coulomb case (which Dollard arranged to yield the "usual" Coulomb amplitude if $V_s = 0$) for any central sufficiently short-range potential, the function $f(k, \theta; \lambda r^{-1} + V_s) - f(k, \theta; \lambda r^{-1})$ has a limit $g(k)$ as $\theta \to 0$ which is the boundary value of a function analytic and polynomially bounded in the cut plane $\mathbf{C}\backslash[0, \infty)$ with $g(\bar{k}) = g(k)$. Moreover, this is not true for any other Dollard dynamics leading to *different* phases. A proof of this conjecture would explain why Gordon's phase is "the right one."

Section XI.10 The idea of formulating the scattering for wave equations as a Hilbert space problem goes back at least as far as M. Birman, "Existence conditions for wave operators," *Izv. Akad. Nauk SSSR Ser. Mat.* **27** (1963), 883–906 (*Amer. Math. Soc. Trans., Ser. 2* **54** (1966), 91–117); and P. Lax and R. Phillips, "The wave equation in exterior domains," *Bull. Amer. Math. Soc.* **68** (1962), 47–49. The necessity of dealing with unitary groups on different spaces was first pointed out by C. Wilcox in "Wave operators and asymptotic solutions of wave propagation problems of classical physics," *Arch. Rational Mech. Anal.* **37** (1966), 37–78. We have mainly followed the general ideas in T. Kato, "Scattering theory with two Hilbert spaces," *J. Functional Analysis* **1** (1967), 342–369. In particular, Theorems XI.75 and XI.76 in case $\mathscr{H}_0 = \mathscr{H}_1$ are contained in Kato's paper including the case where B_0 or B_1 has a nontrivial null space. Kato introduced the notion of equivalence of identification operators and has repeatedly emphasized that on physical grounds certain identification operators are more natural than others.

The details for our sketch of existence and completeness of the wave operators in the case of optical scattering in an inhomogeneous medium (Example 2) can be found in M. Reed and B. Simon, "The scattering of classical waves from inhomogeneous media," *Math. Z.* **155** (1977), 163–180. The construction in the text of the wave operators for Maxwell's equations proves convergence in a norm distinct from the usual energy norm. This can be remedied by looking at the wave equations for the vector potentials. See, for example, the paper just mentioned.

Scattering from obstacles (Example 3) using the point of view of this section is discussed in C. Wilcox, *Scattering Theory for the d'Alembert Equation in Exterior Domains*, Lecture Notes in Math. **442**, Springer-Verlag, New York, Heidelberg, Berlin, 1975; and P. Deift, *Classical Scattering Theory with a Trace Condition*, Princeton Univ. Press, Princeton, New Jersey, 1979. Additional references for scattering from obstacles appear in the notes to Section 11.

The first proofs of asymptotic completeness for acoustical and optical scattering in inhomogeneous media were given independently by M. S. Birman, "Scattering problems for differential operators with perturbations of the space," *Izv. Akad. Nauk SSSR Ser. Mat.* **35** (1971), 440–455; and by J. Schulenberger and C. Wilcox, Completeness of the wave operators for perturbations of uniformly propagative systems," *J. Functional Anal.* **7** (1971), 447–472. Results in certain very special cases were already proven in M. S. Birman, "Existence conditions for wave operators," *Izv. Akad. Nauk SSSR Ser. Mat.* **27** (1963), 883–906 (*Amer. Math. Soc. Trans., Ser. 2* **54** (1966), 91–117). The 1971 Birman paper and the Schulenberger–Wilcox paper required a certain amount of smoothness on the coefficients. The smoothness conditions were removed in V. G. Deič, "Application of the method of nuclear perturbations in two-space scattering theory," *Izv. Vyšš. Učebn. Zaved. Fizika* (1971); and J. Schulenberger, "A local compactness theorem for wave propagation problems of classical physics," *Indiana Univ. Math. J.* **22** (1972), 429–432. The idea that we discuss, using the commutation formula to remove smoothness conditions, is due to P. Deift.

The approach of Schulenberger–Wilcox is different from ours in that they reduce second order wave equations to systems that are first order in the space variables as well as the time variable. For example, in the case of acoustic scattering, if u satisfies (187), then

$$v(x) \equiv \left\langle \frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \frac{\partial u}{\partial x_3}, \frac{\partial u}{\partial t} \right\rangle$$

satisfies

$$\frac{\partial v}{\partial t} = E(x)^{-1}\left(\sum_{i=1}^{3} A_i \frac{\partial}{\partial x_i}\right) v \equiv i\Lambda v \tag{340}$$

where

$$E(x) = \begin{pmatrix} \rho(x) & 0 & 0 & 0 \\ 0 & \rho(x) & 0 & 0 \\ 0 & 0 & \rho(x) & 0 \\ 0 & 0 & 0 & 1/\rho(x)c(x)^2 \end{pmatrix}$$

and the A_i are constant matrices so that

$$\sum_{i=1}^{3} A_i \frac{\partial}{\partial x_i} = \begin{pmatrix} 0 & 0 & 0 & \partial/\partial x_1 \\ 0 & 0 & 0 & \partial/\partial x_2 \\ 0 & 0 & 0 & \partial/\partial x_3 \\ \partial/\partial x_1 & \partial/\partial x_2 & \partial/\partial x_3 & 0 \end{pmatrix}$$

Similarly, one writes the free equation as

$$\frac{\partial v}{\partial t} = E_0^{-1}\left(\sum_{i=1}^{3} A_i \frac{\partial}{\partial x_i}\right) v \equiv i\Lambda_0 v \tag{341}$$

where E_0 is a constant matrix. In his 1966 paper, Wilcox initiated a study of the scattering theory for general first-order systems of the form (340), (341), where:

(i) E_0, $E(x)$, A_i are self-adjoint.
(ii) E_0 and $E(x)$ are strictly positive definite with

$$0 < e_0 \le E(x) \le e_1$$

(iii) The roots of $\det(\lambda E_0 - \sum_{i=1}^{n} A_i p_i)$ have constant multiplicity and constant sign for $p \in \mathbb{R}^n \backslash \{0\}$.
(iv) $E(x) \to E_0$ sufficiently rapidly as $|x| \to \infty$.

Wilcox called systems with a slightly stronger condition "uniformly propagative" and proved the existence of the wave operators. The acoustic equation, Maxwell's equations in isotropic media, and many other classical equations are uniformly propagative. For many results, condition (iii) can be replaced by the weaker condition that $\operatorname{rank}(\sum_1^n A_i p_i)$ be independent of p for $p \in \mathbb{R}\backslash\{0\}$. Such systems of "constant deficit" include Maxwell's equations in general inhomogeneous media. However, completeness was left open since neither the Birman–Belopol'skii theorem, nor Kato's reduction to a single Hilbert space problem was available.

The Birman–Belopol'skii theorem (Theorem XI.13) was proven in M. S. Birman and A. L. Belopol'skii, "The existence of wave operators in scattering theory for a pair of spaces," *Math. USSR-Izv.* **2** (1968), 117–1130. And, in "Some applications of a local criterion for the existence of wave operators," *Soviet Math. Dokl.* **10** (1969), 393–397, M. S. Birman pointed out that the Birman–Belopol'skii theorem can be used to prove completeness in a system of the form (340), (341), *if* $\sum A_i \partial/\partial x_i$ is elliptic. Unfortunately, the first-order systems corresponding to the acoustic wave equation and Maxwell's equations are not elliptic since $\sum A_i p_i$ has zero as an eigenvalue. Schulenberger and Wilcox then showed in their 1971 paper that if one had a coerciveness estimate, then the Birman–Belopol'skii theorem could be extended to the case where there are zero modes. In "Coerciveness inequalities for non-elliptic systems of partial differential equations," *Ann. Mat. Pura Appl.* **88** (1971), 229–305, Schulenberger and Wilcox proved the necessary estimates, thus concluding the proof of completeness for acoustic and optical scattering in inhomogeneous media. Their proof of the coerciveness inequalities was greatly simplified by T. Kato in "On a coerciveness theorem of Schulenberg and Wilcox," *Indiana Univ. J. Math.* **25** (1975), 979–985. See also Deift's book. Birman's 1971 approach to the problem avoided coerciveness estimates but still used local compactness. Recently, in his book, P. Deift has shown that coerciveness inequalities and local compactness can be avoided completely. He uses the more general invariance principle discussed in the notes to Section 3, which says that if

$$\frac{\Lambda_0^n}{(\Lambda_0 + ia)^{2n}} - \frac{\Lambda^n}{(\Lambda + ia)^{2n}} \in \mathscr{I}_1 \tag{342}$$

for each $a \neq 0$, then existence and completeness of the wave operators follows. He is then able to verify (342) since the zero modes are projected out by Λ_0 and Λ.

The Agmon–Kuroda method (see Section XIII.8) has been extended to treat systems like those occurring in this section in T. Kako, "Scattering theory for abstract differential equations of the second order," *J. Fac. Sci. Univ. Tokyo Sect. IA Math.* **19** (1972), 377–392.

For the acoustic wave equation, the problem of the zero modes is an entirely unnecessary difficulty which appears only if one reduces to a first-order equation in the space derivatives. By reducing to first-order only in the time derivative as we did in Example 1, one keeps ellipticity and the Kato reduction-to-one-Hilbert space method or the Birman–Belopol'skii theorem can

be applied directly. In the case of Maxwell's equations one is presented with a nonelliptic system first-order in the space and time variables. But, as indicated in Example 2, this can easily be turned into a second-order (nonelliptic) system. By adding the missing part of the Laplacian one can make the system elliptic by giving the zero modes some nontrivial dynamics. The ellipticity and the Kato reduction theory then give completeness. Since this dynamics decouples from the dynamics of the nonzero modes, the scattering theory for the nonzero modes is not affected. For details, see the Reed-Simon paper. The moral is: If you've got ellipticity, keep it; if you ain't got it, get it.

Trace class results under change of boundary condition go back to M. S. Birman, "Perturbations of the continuous spectrum of a singular elliptic operator under the change of the boundary and boundary conditions," *Vestnik Leningrad. Univ. Mat. Meh. Astronom.* **1** (1962), 22-55. Theorem XI.79 is proven using Wiener integral methods in the Deift-Simon paper quoted in the notes to Section 4; see also B. Simon, *Functional Integration and Quantum Physics*, Academic Press, New York, 1979. Theorems XI.80 and XI.81 are taken from Deift's monograph quoted above; our development follows many of his ideas. His proof of Theorem XI.81, which is very different from our proof of the special case, uses results of A. Calderón, "Lebesgue spaces of differentiable functions and distributions," *Proc. Symp. Pure Appl. Math.* **4** (1961), 33-49, Amer. Math. Soc., Providence, Rhode Island. Deift discusses the more general case of acoustic operators with both obstacles and inhomogeneities. He also remarks that Theorem XI.81 does not handle a case of physical interest where Γ is a piece of hyperplane ("diffraction experiment"). One can, however, modify our proof of Theorem XI.81 to cover this case (Problem 119). Deift develops an alternative theory which works in cases where one can only prove that $R_{\Gamma\cup S;N}$ is compact, a result which is connected with the Rellich-type theorems of Section XIII.14. His idea is (in the notation of the appendix) to prove that $R^2_{\Gamma,N}\chi$ and χR^2_0 are compact and that $R^2_{\Gamma,N}(1-\chi)-(1-\chi)R^2_0$ is trace class. The second result implies the existence of the wave operators, $\Omega^{\pm}(H_{\Gamma;N}, H_0, 1-\chi)$, and the first implies that $1-\chi$ is asymptotically equivalent to the identity.

The idea for Lemma 6 in the proof of Theorem XI.81′ is borrowed from F. Guerra, L. Rosen, and B. Simon, "Boundary conditions for the $P(\varphi)_2$ Euclidean field theory," *Ann. Inst. H. Poincaré Sect. A* **25** (1976), 231-334, who use a similar method in the proof of certain technical estimates relating $R_{\Gamma;N}$ to R_0.

Section XI.11 The basic reference for the approach to scattering theory described in this section is P. D. Lax and R. S. Phillips, *Scattering Theory*, Academic Press, New York, 1967. The representation theorem (Theorem XI.82) which provides the link between incoming and outgoing subspaces and the scattering operator was first stated and proved by Ja. Sinai, "Dynamical systems with countable Lebesgue spectrum, I," *Izv. Akad. Nauk SSSR Ser. Mat.* **25** (1961), 899-924. Sinai deduced the theorem from von Neumann's uniqueness theorem (Theorem XI.84). Lax and Phillips gave a proof from first principles: They first prove the discrete version (Theorem XI.83) and then obtain a spectral representation on $L^2[0, 2\pi; N]$ by the Fourier transform. Using complex analysis and the Cayley transform they obtain a spectral representation on $L^2(-\infty, \infty, N)$ for the continuous case, and then the inverse Fourier transform yields Theorem XI.82. The proof which we give is patterned after ideas in Mackey's imprimitivity theorem. The connection of this theorem to von Neumann's theorem goes back at least to G. W. Mackey, "A theorem of Stone and von Neumann," *Duke Math. J.* **16** (1949), 313-326, and is further discussed in his book *Induced Representations of Groups and Quantum Mechanics*, Benjamin, New York, 1968. References for von Neumann's theorem may be found in the notes to Section VIII.5; an alternative proof is outlined in Problem 30 of Chapter X. Our proof of the lemma to Theorem XI.82 is modeled on von Neumann's celebrated proof of the uniqueness of

Haar measure: J. von Neumann, "The uniqueness of Haar's measure," *Mat. Sb.* **1** (1936), 721-734.

There are connections between ergodic theory and Theorems XI.82 and XI.83 made by Kolmogorov and Sinai, which account for Sinai's interest in the theorems. To see the connection, consider the Baker's transformation (Example 2 of Section VII.4). If D_+ is the space of functions of x alone with $\int f\,dx = 0$, then D_+ can be seen to be an outgoing subspace for U restricted to $\{1\}^{\perp}$, yielding a proof that U is mixing. Theorem XI.82 is relevant for the continuous case. Indeed, one defines a ***K*-system** as a measure space $\langle \Omega, \Sigma, \mu\rangle$ with $\mu(\Omega) = 1$, a one-parameter group T_t of measure preserving transformations and a subalgebra Σ_+ of Σ so that (i) $T_t[\Sigma_+] \subset \Sigma_+$ for $t > 0$; (ii) the largest σ-algebra contained in all $T_t[\Sigma_+]$ is $\{\varnothing, \Omega\}$; (iii) the smallest σ-algebra containing all the $T_t[\Sigma_+]$ is Σ. If one takes $\mathscr{H} = \{f \in L^2 \mid \int f\,d\mu = 0\}$, $D_+ = \{f \in \mathscr{H} \mid f \text{ is } \Sigma_+ \text{ measurable}\}$ and $U(t)f = f \circ T_t^{-1}$, then D_+ is an outgoing subspace and, in particular T_t is mixing.

In their book, Lax and Phillips use the scattering of acoustical waves by an obstacle with Dirichlet boundary conditions (Example 3) as the main example to illustrate the application of their general theorems. Their theory also applies to Neumann and certain other boundary conditions. We have used scattering from inhomogeneous media to illustrate the general theory in order to facilitate comparison with the techniques of Section 10. Because of interest in the connection between the geometry of the obstacle, local energy decay, and the poles of the scattering operator (see below), obstacle scattering in homogeneous media has been the main problem discussed in the literature, though many authors have noted that their results extend to inhomogeneous media. The inhomogeneous case is explicitly treated using the Lax-Phillips theory in J. LaVita, J. Schulenberger, and C. Wilcox, "The scattering theory of Lax and Phillips and wave propagation problems of classical physics," *ONR Tech. Rep.* **16** (1971).

Theorem XI.89 is a special case of a general theorem of Y. Foures and I. Segal, "Causality and analyticity," *Trans. Amer. Math. Soc.* **78** (1955), 385-405. A proof of Fatou's theorem may be found in Chapter 11 of P. Duren, *Theory of H^p Spaces*, Academic Press, New York, 1970. The original idea goes back to P. Fatou, "Series trigonométriques et séries de Taylor," *Acta Math.* **30** (1906), 335-400, who treated the case of a bounded analytic function in a disk. The scattering operator $s(z)$ in the Lax-Phillips book is analytic in the *lower* half-plane because they use the plus sign for the Fourier transform while we use the minus sign. For proofs of Theorems XI.90 and XI.91 which connect the poles of $s(z)$ to the spectrum of B, see the book by Lax and Phillips. The statements of results are different since they write semigroups as $Z(t) = e^{Bt}$ while we write semigroups as e^{-Bt}. Thus their B has spectrum in the left half-plane and ours has spectrum in the right half-plane.

The poles of the scattering operator are closely connected with physical observation, so it is important to investigate their positions in the lower half-plane. According to Theorem XI.90, this problem reduces to studying $\sigma(B)$. By using a functional calculus for B, the conclusion of Theorem XI.91 can be strengthened in various ways by adding more hypotheses:

Theorem Suppose that the hypotheses of Theorem XI.91 hold. Then,

(a) If for some T, $\|Z(T)\| = a < 1$, then

$$\sigma(B) \subset \left\{ z \,\middle|\, \operatorname{Re} z \geq -\frac{\ln a}{T} \right\}$$

(b) If $Z(T)$ is compact for some T, then for every $c > 0$ there are only finitely many points of $\sigma(B)$ in the set $\{z \mid \operatorname{Re} z < c\}$.

(c) If for some T the range of $Z(T)$ lies in $D(B)$, then there exist $a \in \mathbb{R}$, $b > 0$ so that

$$\sigma(B) \subset \left\{ z \,\middle|\, \operatorname{Re} z > a + b \ln |z| \right\}$$

Conditions (a) and (b) were given by Lax and Phillips in their book. They also showed that condition (b) implies the existence of an asymptotic series in the energy norm of a solution in a bounded region; the series is a sum of exponentials with rates depending on positions of the poles. Because of this, condition (b) is particularly important to verify in applications. Condition (c) was stated and verified in P. Lax and R. S. Phillips, "A logarithmic bound on the location of the poles of the scattering matrix," *Arch. Rational Mech. Anal.* **40** (1971), 268–280, for the equation $u_{tt} - c(x)^2 \Delta u - q(x)u = 0$ under a variety of hypotheses. C. S. Morawetz and D. Ludwig, "The generalized Huygens' principle for reflecting bodies," *Comm. Pure Appl. Math.* **22** (1969), 189–205, prove a general Huygens' principle for the propagation of singularities and energy decay for scattering from a convex body (Dirichlet boundary conditions) and use the result to verify (b). Another proof of (b) using their Huygens' principle appears in R. S. Phillips, "A remark on the preceding paper of C. S. Morawetz and D. Ludwig," *Comm. Pure Appl. Math.* **22** (1969), 207–211. In C. S. Morawetz, "The decay of solutions of the exterior initial-boundary value problem for the wave equation," *Comm. Pure Appl. Math.* **14** (1961), 561–568, and "The limiting amplitude principle," *Comm. Pure Appl. Math.* **15** (1962), 349–361, it was shown that the energy decays uniformly like t^{-1} in bounded regions exterior to a star-shaped obstacle; and P. Lax, C. S. Morawetz, and R. S. Phillips, "Exponential decay of solutions of the wave equation in the exterior of a star-shaped obstacle," *Comm. Pure Appl. Math.* **16** (1963), 477–486, then showed that this implies an exponential rate of decay. This in turn implies that $\|Z(t)\varphi\| \leq ce^{-\alpha t}\|\varphi\|$, so (a) holds in the case of a star-shaped obstacle.

Notice that our verification of the hypotheses of Theorem XI.91 in Example 3 used the fact that the local energy decays, but uniformity was not required nor were any special geometric conditions required of the obstacle. On the other hand, to get uniform decay one would expect some geometric condition (as the above titles suggest) since if the obstacle is too badly dented, it should be possible to trap energy in its vicinity for arbitrarily long times by appropriate choices of initial conditions. In their book, Lax and Phillips conjecture that if the sojourn times of light rays in the neighborhood of the obstacle are unbounded above, then $\|Z(t)\| = 1$ for all t. The conjecture was verified by J. Ralston in "Solutions of the wave equation with localized energy," *Comm. Pure Appl. Math.* **22** (1969), 807–823. In "Trapped rays in spherically symmetric media and poles of the scattering matrix," *Comm. Pure Appl. Math.* **24** (1971), 571–582, Ralston shows that the same is true in the inhomogeneous case if $c(x)$ wiggles too much at ∞. Lax and Phillips also conjectured that if the sojourn times are bounded, then $Z(t)$ is eventually compact, which in particular would imply that $\|Z(t)\|$ is eventually less than one by (223). This weaker form of the conjecture has been proven in C. Morawetz, J. Ralston, and W. Strauss, "Decay for solutions of wave equations outside of non-trapping obstacles," *Comm. Pure Appl. Math.* **30** (1977), 447–508. This connection between the geometry of the obstacle and the poles of the scattering operator via energy decay estimates is one of the most beautiful aspects of the Lax–Phillips method. In this connection, C. S. Morawetz and D. Ludwig, "An inequality for the reduced wave operator and the justification of geometrical optics," *Comm. Pure Appl. Math.* **21** (1968), 187–203, show that the formal solution of the scattering problem given by geometrical optics is asymptotic to the exact solution given by the Lax–Phillips theory. For other results on the position of the poles of $s(z)$, see P. Lax and R. S. Phillips, "Decaying modes for the wave equation in the exterior of an obstacle," *Comm. Pure Appl. Math.* **22** (1969), 737–787; and "On the scattering frequencies for the Laplace operator for exterior domains," *Comm. Pure Appl. Math.* **25** (1972), 85–101.

The application of their method to quantum scattering is described by Lax and Phillips in their book and further developed in P. D. Lax and R. S. Phillips, "The acoustic equation with an indefinite energy form," *J. Functional Analysis* **1** (1967), 37–83. See also C. Dolph, J. McLeod, and D. Thoe, "The analytic continuation to the unphysical sheet of the resolvent kernel and the scattering operator associated with the Schrödinger equation," *J. Math. Anal. Appl.* **16** (1966), 311–332.

In their book Lax and Phillips also present two proofs (one due to M. Schiffer) that the obstacle (Dirichlet conditions) is uniquely determined by the scattering operator. This has been extended by A. Majda who shows in "High frequency asymptotics for the scattering matrix and the inverse problem of acoustical scattering," *Comm. Pure Appl. Math.* **29** (1976), 261–291, and "A representation formula for the scattering operator and the inverse problem for arbitrary bodies" *Comm. Pure Appl., Math.* **30** (1977), 165–194, that a convex hull obstacle is already determined through an explicit formula by the high frequency asymptotics of the kernel $k(\theta, w; \sigma)$ of $I - \hat{S}$. Majda's results have been extended by P. Lax and R. S. Phillips, "Scattering of sound waves from an obstacle," *Comm. Pure Appl. Math.* **30** (1977), 195–233.

The Lax–Phillips approach has been extended and applied to a variety of other situations than those we have discussed: For even dimensions, see P. Lax and R. S. Phillips, "Scattering theory for the acoustic equation in an even number of space dimensions," *Indiana Univ. Math. J.* **22** (1972), 101–134. For symmetric hyperbolic systems with conserved energy, see P. D. Lax and R. S. Phillips, "Scattering theory," *Rocky Mountain J. Math.* **1** (1971), 173–223. For dissipative hyperbolic systems, see P. D. Lax and R. S. Phillips, "Scattering theory for dissipative hyperbolic systems," *J. Functional Analysis* **14** (1973), 172–236; and C. Foias, "On the Lax–Phillips nonconservative scattering theory," *J. Functional Analysis* **19** (1975), 272–301. For moving obstacles, see J. Cooper and W. Strauss, "Energy boundedness and decay of waves reflected off a moving boundary," *Indiana Univ. Math. J.* **25** (1976), 671–690. For an application to transport phenomena, see P. D. Lax and R. S. Phillips, "Scattering theory for transport phenomena," in *Functional Analysis* (B. Gelbaum, ed.), Thompson, 1967. Scattering in certain non-Euclidean geometries which leads to S-matrices that are connected to automorphic functions are studied in L. Faddeev and B. S. Pavlov, "Scattering theory and automorphic functions," *Sem. Steklov Inst. Math. Leningrad* **27** (1972), 161–193, and P. Lax and R. S. Phillips, *Scattering Theory for Automorphic Functions*, Ann. Math. Stud. **87**, Princeton Univ. Press, Princeton, New Jersey, 1976.

The twisting trick of the appendix is due to E. B. Davies and B. Simon in their paper quoted in the notes to Section 4. They discuss the Neumann boundary condition case and several other applications.

Section XI.12 The material in this section is based on three papers: J. Hejtmanek, "Scattering theory of the linear Boltzmann operator," *Comm. Math. Phys.* **43** (1974), 109–120; B. Simon, "Existence of the scattering matrix for the linearized Boltzmann equation," *Comm. Math. Phys.* **41** (1975), 99–108; and J. Voigt, "On the existence of the scattering operator for the linear Boltzmann equation," *J. Math. Anal. Appl.* **58** (1977), 541–558. See also V. Protopopescu, "On the scattering matrix for the linear Boltzmann equation," *Rev. Roumaine Phys.* **21** (1976), 991–994.

Hejtmanek (whose paper was the first to appear in preprint form) isolated the problem and proved the basic solvability result in Theorem XI.93 including assertions (a)–(c) and Theorem XI.94. Simon introduced the lemma appearing before Theorem XI.94, proved Theorem XI.95 under the stronger hypothesis (diam $D)(M(\sigma_a) + M(\sigma_p)) < 1$, and proved Theorem XII.96 under this same hypothesis. Simon remarks that these ideas are closely related to the theory of smooth perturbations discussed in Section XIII.7. Simon's paper also contains an example

showing that the dynamics may not be invertible on L^1_+. Voigt proved the estimate in Theorem XI.93d and Theorems XI.95 and XI.96 under the hypotheses we use. He also extended these results to some cases of noncompact support and gave an example of a regular subcritical pair for which $\tilde{\Omega}^-$ fails to exist.

The general (that is, nonlinear) Boltzmann equation was suggested by L. Boltzmann, "Uber die Aufstellung und Integration der Gleichungen, welche die Molekularbewegung in Casen bestimmen," *Sitz. Wien.* **74** (1876), 503. For recent discussion of mathematical problems associated with this equation, see E. G. D. Cohen and W. Thirring. *The Boltzmann Equation*, Springer; Vienna, 1973. The linearized Boltzmann equation has been used extensively to study phenomena very different from those we discuss: for those transport phenomena associated with reactors, see I. Bell and S. Glasston, *Nuclear Reactor Theory*, Van Nostrand, Princeton, New Jersey, 1970; for transport phenomena in stars, D. Mihalas, *Stellar Atmospheres*, Freeman, San Francisco, 1970.

Section XI.13 The first results on the scattering theory of the equation

$$u_{tt} - \Delta u + m^2 u = -gu^3 \tag{343}$$

were proven in I. Segal, "Quantization and dispersion for nonlinear relativistic wave equations," *Proc. Conf. Mathematical Theory of Elementary Particles (Dedham, Mass. 1965)*, pp. 79–108, MIT Press, Cambridge, Massachusetts. Segal showed that for all sufficiently nice solutions u_- of the free equation, there is a solution u of (343) such that $u_- - u \to 0$ as $t \to -\infty$. Similarly for each u_+, a u exists. Thus, Segal constructed the wave operators $\Omega^\pm$ on certain sets of nice data. In "Dispersion for nonlinear relativistic wave equations," *Ann. Sci. École Norm. Sup.* **1** (1968), 459–497, Segal showed that if u_- and u_+ are small (or g is small), then $\Omega^\pm$ can be inverted so the scattering operator exists for small data. This paper contains most of the small data scattering ideas we have presented. Small data methods were then applied by J. Chadam to more general equations in "Asymptotics for $\Box u = m^2 u + G(x, t, u, u_x, u_t)$, I, II," *Ann. Scuola Norm. Sup. Pisa Fis. Mat.* **26** (1972), 33–65, 67–95; and by W. von Wahl for the case $m = 0$ in "Uber die klassische Lösbarkeit des Cauchyproblems für nichtlineare Wellengleichungen bei kleinen Anfangswerten und das asymptotische Verhalten der Lösungen," *Math. Z.* **114** (1970), 281–299. The abstract low energy scattering theory that we present follows closely the outline in W. Strauss, "Nonlinear scattering theory," in *Scattering Theory in Mathematical Physics* (J. Lavita and J.-P. Marchand, eds.), Reidel, Dordrecht, The Netherlands, 1974. The proof that we give of Theorem XI.98 includes several additional improvements of Strauss.

Our proof of Theorem XI.101 is closely patterned after the original proof of W. Strauss, "Decay and asymptotics for $\Box u = F(u)$," *J. Functional Analysis* **2** (1968), 409–457. The idea of proving a decay estimate by integrating by parts and identifying positive terms in a conserved quantity goes back at least to C. Morawetz, "The limiting amplitude principle," *Comm. Pure Appl. Math.* **15** (1963), 349–361. Asymptotic completeness for (343) for the case $m > 0$ is much harder to prove than in the case $m = 0$. Although there is a broken conformal charge, similar to that in Problem 153, the source term is positive, which ruins the decay estimate. For the $m > 0$ case, where $g = g(x)$ is small at ∞, Strauss constructed Ω^+ and Ω^- in "Decay of solutions of hyperbolic equations with localized nonlinear terms," *Symposia Mathematica*, Vol. VII, *Probleme di Evoluzione*, Instituto Nazionale di Alta Matematica (Roma), Academic Press, New York, 1971, 339–355. Then C. Morawetz and W. Strauss proved asymptotic completeness for $m > 0$, g a positive constant, in "Decay and scattering of solutions of a nonlinear relativistic wave equation," *Comm. Pure Appl. Math.* **25** (1972), 1–31. Their proof, which is quite difficult, successively improves a weak decay estimate which had previously been obtained by C. Morawetz in "Time decay for the Klein–Gordon equation," *Proc. Roy. Soc. London Ser. A* **30G** (1968), 291–296. An abstract version of their proof appears in M. Reed, "Construction of the scattering operator for abstract nonlinear wave equations," *Indiana Univ. Math. J.* **25** (1976), 1017–1027. Further properties of the scattering operator are proven in C. Morawetz and W. Strauss, "On a nonlinear scattering operator," *Comm. Pure Appl. Math.* **26** (1973), 47–54.

Asymptotic completeness for the nonlinear Schrödinger equation

$$i\, du/dt = (-\Delta + m)u + f(u)$$

for various nonlinear terms $f(u)$ has been proven in J. E. Lin and W. Strauss, "Decay and scattering of solutions of the nonlinear Schrödinger equation," *J. Functional Analysis* **30** (1978), and in a series of papers by J. Ginibre and G. Velo, "On a class of non-linear Schrödinger equations," I and II, *J. Functional Analysis*, to appear; III, *Ann. Institut Poincaré* **28** (1978), 287–316. To obtain the necessary a priori decay estimate, Ginibre and Velo use a broken invariance analogously to the use of the broken conformal invariance described in Problem 153.

There is an extensive literature on this subject. For references and further discussion, see M. Reed, *Abstract Non-linear Wave Equations*, Lecture Notes in Mathematics **507**, Springer-Verlag, New York, Heidelberg, Berlin, 1976, and Strauss's "Non-linear scattering theory" lectures referred to above, and his "Invariant wave equations" lectures referred to below.

A discussion of bound states in nonlinear systems and, in particular, the details of the example can be found in W. Strauss, "Existence of solitary waves in higher dimensions," *Commun. Math. Phys.* **55** (1977), 149–162, where references are given to earlier work.

There has been extensive study of a special class of equations, including the Korteweg-de Vries equation and the sine-Gordon equation, which have bound states with very special properties. Namely, there is no scattering between channels. That is, a state that looks like n solitons at $t = -\infty$ will also look like n solitons at $t = +\infty$. Indeed, the velocities of the solitons will even be the same. For an introduction to the literature, see C. Scott, F. Chu, D. McLaughlin, "The soliton: A new concept in applied science," *Proc. IEEE* **61** (1973), 1443–1483; and *Nonlinear Wave Motion* (A. Newell, ed.), Lectures in Applied Mathematics **15**, Amer. Math. Soc., Providence, Rhode Island, 1974

Noether's theorem goes back to E. Noether, "Invariante Variationsprobleme," *Nachr. Akad. Wiss. Göttingen Math-Phys.* (kl. II) (1918), 235–257. These ideas have become a standard part of classical field theory; see, for example the treatment in N. Bogoliubov and D. Shirkov, *Introduction to the Theory of Quantized Fields*, Wiley (Interscience), New York, 1959. That invariants of the dynamics are connected with groups of transformations commuting with the dynamics is an idea that is familiar from classical and quantum mechanics. Let $T_t^{(H)}$ be the flow on phase space generated by a Hamiltonian $H(p, q)$ through the Hamilton equations (X.153). If $T_t^{(f)}$ is the flow generated by $f(p, q)$ and $T_t^{(H)} T_s^{(f)} = T_t^{(f)} T_s^{(H)}$, then f is invariant under $T_t^{(H)}$, that is, $f(T_t^{(H)}\langle p, q\rangle) = f(p, q)$. In quantum mechanics, let H be the Hamiltonian and A another self-adjoint operator. If e^{-isH} and e^{-itA} commute, then the spectral measures of A are invariant under e^{-itH}, that is,

$$(E_\Omega^{(A)} e^{-itH}\varphi, e^{-itH}\varphi) = (E_\Omega^{(A)}\varphi, \varphi) \qquad \text{for all } \varphi \text{ and } t$$

Notice, however, two things about the classical field theory case. First, it is more convenient to work in the Lagrangian formulation than in the Hamiltonian formulation. Secondly, the conserved quantities appear as the integrals of local densities.

For a different but related approach to finding conserved quantities and many references, see W. Strauss's lectures, "Nonlinear invariant wave equations," in *Invariant Wave Equations*, Springer Lecture Notes in Physics **73** (1978), 197–249.

The group of fractional linear transformations on $\mathbb{C}$ is generated, geometrically, by rotations, translations, dilations, and inversion on $\mathbb{R}^2$. Analogously, the group of transformations of $\mathbb{R}^4$

generated by rotations, translations, dilations, and the inversion $x \to x/x \cdot x$ is called the conformal group because it too preserves angles. If we continue t to it, the rotation group becomes the Lorentz group and the inversion becomes the Lorentz inversion; this is the group that physicists usually refer to as the conformal group. It preserves angles in the Lorentz inner product.

Section XI.14 The notion of magnons was first developed in the physics literature in connection with theories of ferromagnetism. We do not intend to give any complete discussion of the rather extensive literature on the subject or on the Heisenberg model in general, but we mention the instructive article of F. Dyson, "General theory of spin-wave interactions," *Phys. Rev.* **102** (1956), 1217–1230; and a collection of reprints on *Ferromagnetism* published by the Physical Society of Japan.

The basic ideas for scattering in the zero-temperature Heisenberg model are due to G. J. Watts, "Theory of spin-wave scattering," Ph.D. Thesis, Bedford College, 1973; and K. Hepp, "Scattering theory in the Heisenberg ferromagnet," *Phys. Rev. B* **5** (1972), 95–97. A comprehensive review can be found in R. F. Streater, "Spin-wave scattering" in *Scattering Theory in Mathematical Physics* (J. A. LaVita and J. P. Marchand, eds.), pp. 273–298, Reidel, Dordrecht, The Netherlands, 1974.

Bound states of magnons are discussed in J. G. Hanus, "Bound states in the Heisenberg ferromagnet," *Phys. Rev. Lett.* **11** (1963), 336–337; and M. Wortis, "Bound states of two spin waves in the Heisenberg ferromagnet," *Phys. Rev.* **132** (1963), 85–97.

One can study magnon scattering in the one-dimensional Heisenberg model at a much more detailed level since it is possible to obtain many formulas in closed form. In particular, for each n, there is exactly one n-magnon bound state. The reason this model is so tractable is that, like solitons in one dimension, the spin waves do not scatter off one another, nor is there transfer of momentum. For more details, see L. Thomas, "Ground state representation of the infinite one-dimensional Heisenberg ferromagnet, I," *J. Math. Anal. Appl.* **59** (1977), 392–414; D. Babbitt and L. Thomas, "Ground state representation of the infinite one-dimensional Heisenberg ferromagnet, II. An explicit Plancherel formula," *Comm. Math. Phys.* **54** (1977), 255–278; and D. Babbitt and L. Thomas, "Ground state representation of the infinite one-dimensional Heisenberg ferromagnet, III. Scattering theory," *J. Mathematical Phys.*, **19** (1978), 1699–1704.

The Hilbert space that we constructed in the infinite volume case can also be realized as an infinite tensor product. Let

$$D_0 = \left\{ \bigotimes_{\alpha \in \mathbf{Z}^3} v_\alpha \,\middle|\, v_\alpha \in \mathbf{C}^2, \text{ all but finitely many } v_\alpha \text{ equal } \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$$

where we define a linear structure so that $\otimes v_\alpha$ is linear in each v_α when all the others are fixed. For v and w in D_0 with $v = \otimes v_\alpha$, $w = \otimes w_\alpha$, we define

$$(v, w) = \prod_{\alpha \in \mathbf{Z}^3} (v_\alpha, w_\alpha)_{\mathbf{C}^2} \tag{344}$$

The product makes sense since all but finitely many terms are equal to one. Moreover, (344) extended to be sesquilinear can be shown to define an inner product on D_0 (Problem 136). Then, the completion of D_0 in the inner product is a Hilbert space which is one of an uncountable set of distinct tensor products we can construct by replacing $\binom{0}{1}$ by different sequences. This space is isomorphic to $\mathscr{H}$ under the map $\psi(\{\alpha_\beta\}) \mapsto \otimes v_\beta$ where $v_\beta = \binom{0}{1}$ (respectively, $\binom{1}{0}$) if $\alpha_\beta = 0$ (respectively, 1). Infinite tensor products were introduced by J. von Neumann in "On infinite direct products," *Compositio Math.* **6** (1938), 1–77. For a summary, see the appendix in M. Reed, "Self-adjointness in infinite tensor product spaces," *J. Functional Analysis* **5** (1970), 94–124.

Section XI.15 The mathematical treatment of quantum field scattering in an external field has its roots in the work of R. Feynman, "The theory of positrons," *Phys. Rev.* **76** (1949), 749–759; A. Salam and P. Matthews, "Fredholm theory of scattering in a given time-dependent field," *Phys. Rev.* **90** (1953), 690–695; and J. Schwinger, "Theory of quantized fields, IV, V," *Phys. Rev.* **92** (1953), 1283–1299; **93** (1954), 615–628. All four papers deal with electron–positron scattering in a given external classical electromagnetic field. Feynman wrote down successive approximations to certain scattering amplitudes in terms of classical propagators and discussed the connection between his formulas, the hole theory of Dirac, and second quantization. The papers of Salam–Matthews and Schwinger write down what was implicit in Feynman's paper, namely, Dyson-type expansions for the scattering operator in terms of the in field and the external field, and study the convergence of the expressions for certain matrix elements.

The realization of Yukawa field theories as an integral over external fields was developed on a formal level by A. Salam and P. Matthews, "The Green's functions of quantized fields," *Nuovo Cimento* **12** (1954), 563–565; "Propagators of quantized fields," *Nuovo Cimento* **2** (1955), 120–134. For the two-dimensional theory, the formalism was put on a rigorous footing by E. Seiler, "Schwinger functions for the Yukawa model in two dimensions with space-time cutoff," *Comm. Math. Phys.* **42** (1975), 153–182. See also, E. Seiler and B. Simon, "Nelson's symmetry and all that in the $(\text{Yukawa})_2$ and $(\varphi^4)_3$ field theories," *Ann. Physics* **97** (1976), 476–518. This formalism has been responsible for much recent progress including verification of the Wightman axioms for small coupling.

The first attempt to develop the entire mathematical apparatus for external field problems in a fully rigorous way was made by A. Capri, "Electron scattering in a given time-dependent electromagnetic field," *J. Mathematical Phys.* **10** (1969), 575–580. Capri pointed out that the construction of the dynamics for the field could be completely reduced to constructing the analogous classical dynamics. However, Capri's proof of the existence of the out-vacuum was inconclusive. This difficulty was remedied in B. Schroer, R. Seiler, and J. Swieca, "Problems of stability for quantum fields in external time-dependent potentials," *Phys. Rev. D* **2** (1970), 2927–2937, where spins other than $\frac{1}{2}$ are also discussed. The development of the theory in the spin zero (coupling of (278)) and spin $\frac{1}{2}$ cases was summarized in R. Seiler, "Quantum theory of particles with spin zero and one half in external fields," *Comm. Math. Phys.* **25** (1972), 127–151. We have followed in part the presentation in Seiler's paper.

Additional references on the external field problem include: J. Bellissard, "Quantized fields in interaction with external fields; I. Exact solutions and perturbation expansion; II. Existence theorems," *Comm. Math. Phys.* **41** (1975), 235–266; **46** (1976), 53–74; P. Bongaarts and S. Ruijsenaars, "The Klein paradox as a many particle problem," *Ann. Physics* **101** (1976), 289–318; J. M. Chadam, "Unitarity of dynamical propagators of perturbed Klein-Gordon equations," *J. Mathematical Phys.* **9** (1968), 386–396; W. Hochstenbach, "Field theory with an external potential," *Comm. Math. Phys.* **51** (1976), 211–217; M. Klaus and G. Scharf, "The regular external field problem in quantum electrodynamics," *Helv. Phys. Acta* **50** (1977), 779–802 and "Vacuum polarization in Fock space," *Helv. Phys. Acta* **50** (1977), 803–814; L. E. Lundberg, "Relativistic quantum theory for charged spinless particles in external vector fields," *Comm. Math. Phys.* **31** (1973), 295–316; J. Palmer, "Scattering automorphisms of the Dirac field," *J. Functional Analysis*, to appear, and "Symplectic groups and the Klein–Gordon field," *J. Math. Anal. and Appl.*, to appear; S. Ruijsenaars, "Charged particles in external fields; I. Classical theory; II. The quantized Dirac and Klein Gordon theories," *J. Mathematical Phys.* **18** (1977), 720–737, *Comm. Math. Phys.* **52** 1977), 267–294, and the collection of articles in *Invariant Wave Equations* (G. Velo and A. S. Wightman, eds.), Springer Lecture Notes in Physics **73**, Berlin, Heidelberg, New York, 1978.

Theorem XI.108 is due to D. Shale, "Linear symmetries of free boson fields," *Trans. Amer. Math. Soc.* **103** (1962), 149–167. The analogous theorem for fermions was proven in D. Shale and W. Stinespring, "Spinor representations of infinite orthogonal groups," *J. Math. Mech.* **14** (1965), 315–322. Both papers depend on results in I. Segal, "Distributions in Hilbert space and canonical systems of operators," *Trans. Amer. Math. Soc.* **88** (1958), 12–41. There is a large literature on Bogoliubov transformations; see, for example, R. Powers and E. Størmer, "Free states of the canonical anti-commutation relations," *Comm. Math. Phys.* **16** (1970), 1–33; K. Fredenhagen, "Implementation of automorphisms and derivations of the CAR algebra," *Comm. Math. Phys.* **52** (1977), 255–266; and G. Labonté, "On the nature of strong Bogoliubov transformations for fermions," *Comm. Math. Phys.* **36** (1974), 59–72 for the fermion case, P. Kristensen, L. Mejlbo, and E. T. Poulsen, "Tempered distributions in infinitely many dimensions, III: Linear transformations of field operators," *Comm. Math. Phys.* **6** (1967), 29–48; A. Klein, "Quadratic expressions in a free Boson field," *Trans. Amer. Math. Soc.* **181** (1973), 439–456; and F. Berezin, *The Method of Second Quantization*, Academic Press, New York, 1966, for the Boson case; and S. Ruijsenaars, "On Bogoliubov transformations, I, II," *J. Mathematical Phys.* **18** (1977), 517–526, and *Ann. Phys.* (to appear).

There is an equivalent formalism for Bogoliubov transformations called the symplectic transformation approach. This is the approach used by Segal and Shale, in particular. It is more compact, mathematically more elegant, and it makes contact with various problems in group representations and number theory; however, explicit calculations of the kind we make in the text are often easier in the Bogoliubov formalism.

To describe the symplectic transformation approach, we recall that the Segal field operator $\Phi_S(f)$ of Section X.7 was defined over any complex Hilbert space $\mathscr{H}$ but that $f \to \Phi_S(f)$ was only *real* linear. The canonical commutation relations took the form

$$[\Phi_S(f), \Phi_S(g)] = i\,\mathrm{Im}(f, g)_{\mathscr{H}}$$

A **symplectic** transformation is a *real* linear map T: $\mathscr{H} \to \mathscr{H}$ so that

$$\mathrm{Im}(Tf, Tg) = \mathrm{Im}(f, g) \tag{345a}$$

If one lets T^t be the adjoint of T as a map on the real Hilbert space $\mathscr{H}_r$ with inner product $(f, g)_r = \mathrm{Re}(f, g)$, then (345a) is equivalent to

$$T^t J T = J \tag{345b}$$

where J is multiplication by i. If one picks a complex conjugation C, then one can write $\mathscr{H}_r = \mathscr{K} \oplus J\mathscr{K}$ where $\mathscr{K}$ is the real subspace $\mathscr{K} = \{\varphi \,|\, C\varphi = \varphi\}$. In terms of this direct sum $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$ and (345b) can be recognized as the usual symplectic transformation condition if $\dim \mathscr{K} < \infty$. The symplectic transformations induce a natural transformed field

$$(\mathscr{T}\Phi)_S(f) = \Phi_S(Tf) \tag{346}$$

Since

$$a^\dagger(f) = \frac{1}{\sqrt{2}}[\Phi_S(f) - i\Phi_S(Jf)]$$

$$a(Cf) = \frac{1}{\sqrt{2}}[\Phi_S(f) + i\Phi_S(Jf)]$$

we see that (346) is equivalent to (301) if we take

$$(\mathscr{T}\Phi)_S(f) = \frac{1}{\sqrt{2}}[a_B^\dagger(f) + a_B(Cf)]$$

$$B_+ = \frac{1}{2}[T - JTJ], \qquad B_- = \frac{C}{2}[T + JTJ] \tag{347}$$

Notice that $B_\pm$ are complex linear and that (298) is equivalent to (345). The inverse formulas (299), (300) are equivalent to $T^{-1} = -JT^tJ$ which holds if T is invertible (a priori it may have only a left inverse).

Shale's original implementability theorem says that if T is an invertible symplectic transformation, then there exists a unitary U_T so that

$$U_T \Phi_S U_T^{-1} = (\mathscr{T}\Phi)_S$$

if and only if $T^tT - 1$ is Hilbert-Schmidt. But, by (347) and (345b),

$$T^tT - 1 = 2T\,CB_- \tag{348}$$

so that Shale's criterion is equivalent to the $B_- \in \mathscr{I}_2$ criterion we state since $2T^tC$ is invertible. Shale's proof is somewhat different from that we give and proceeds by first writing a real polar decomposition $T = Q|T|$, with $|T| = \sqrt{T^tT}$. The orthogonal symplectic transformation Q is explicitly implementable by the operator $\Gamma(Q)$ equal to $Q \otimes \cdots \otimes Q$ on $\Gamma_n(\mathscr{H})$; in Bogoliubov transform language, $B(Q)_- = 0$ by (348) so $B(Q)_+$ is unitary and $\Gamma(U)a^\dagger(f)\Gamma(U)^{-1} = a^\dagger(Uf)$ trivially. Thus, one need only prove the theorem in the case $T > 0$. In that case, one can formally realize T as a scale transformation S_T on Q space and write an explicit formula for a unitary inducing T by $(Uf)(q) = N_T(q)f(S_Tq)$ where $N_T(q)^2$ is a Jacobian for the change of variables. The condition $T^tT - 1 \in \mathscr{I}_2$ is needed to show that $N_T(q)$ is well defined.

Shale's theorem in case $T^t = T$ is equivalent to asking when two Gaussian processes are mutually absolutely continuous; this is discussed in Section I.6 of B. Simon, *The $P(\varphi)_2$ Euclidean (Quantum) Field Theory*, Princeton Univ. Press, Princeton, New Jersey, 1974. These results are well known in the probability literature and predate the work of Shale; see J. Feldman, "Equivalence and perpendicularity of Gaussian Processes," *Pacific J. Math.* **8** (1958), 699–708, and J. Hajek, "On a property of the normal distribution of any stochastic process," *Czech. Math. Z.*, **8** (1958), 610–618 (Selected translation in *Math. Stat. Prob.* **1** (1961) 245–256).

For the coupling that we used in the section, we could have carried through the theory with a single Hermitian scalar field. For other couplings it is often necessary to use the charged field.

The smoothness hypothesis on $V(x, t)$ which we made in the section were convenient but not crucial. However, some kind of smallness condition on V as $|x| \to \infty$ and $|t| \to \infty$ is necessary for our simple approach to go through. First, suppose that $V(x, t) = \alpha(t)$ and that $\alpha(\cdot)$ has compact support in t, that is, we turn on and then turn off a constant scalar field. Then we can define the interacting dynamics as in the section obtaining at each time t a representation of the canonical commutation relations $a(x, t)$, $b^\dagger(x, t)$; but we cannot expect this dynamics to be unitarily implemented since turning on $\alpha(t)$ is the same as changing the mass. And, even for free fields, changing the mass means changing the representation of the canonical commutation relations (Theorem X.46). The physical reason for this is that since the potential is infinitely extended, it can create infinitely many pairs in a finite time. On the other hand, suppose that $V(x, t) = \beta(x)$ is independent of time. Then even if $\beta(x)$ is localized in space, it is not clear how to define the out-fields or the out-dynamics. And, certainly one would not expect in general the out representation of the canonical commutation relations to be unitarily equivalent to the in

fields since the potential has time to create infinitely many pairs. Using the machinery of Banach algebras, P. Bongaarts in "The electron-positron field, coupled to external electromagnetic potentials, as an elementary C^* algebra theory," *Ann. Physics* **56** (1970), 108–139, has shown how to define the outfields in the case of the Dirac equation in a static external field. For certain very special cases he obtains unitary implementability. These difficulties in the *linear* external field problems, where there are no problems of multiplying operator-valued distributions together, show how hard the dynamics for fully nonlinear field theories really are.

There has been a considerable amount of work on the external field problem for higher spin equations ($s > 1$) where, in all known cases, there are additional difficulties. First, it is sometimes difficult to choose an appropriate positive definite inner product on the space of solutions—the positive definiteness is needed for second quantization. If one changes the inner product to force it to be positive definite, then one loses the commutation relations for the corresponding propagated field. Secondly, G. Velo and D. Zwanziger in "Propagation and quantization of Rarita-Schwinger waves in an external electromagnetic potential," *Phys. Rev.* **186** (1969), 1337–1341, and "Noncausality and other defects of interaction Lagrangians for particles of spin one and higher," *Phys. Rev.* **188** (1969), 2218–2222, discovered that certain formally Lorentz invariant equations have a noncausal propagation. What they showed was this: Call a fundamental solution "causal" if it has support in the forward light cone and "weakly causal" if it decays faster than any power in spacelike directions. Velo and Zwanziger showed for certain equations that *if* they have a weakly causal fundamental solution, then it is *not* causal. Recently L. Gårding has shown that there are equations and external fields for which no weakly causal fundamental solutions exist. There are still further diseases. Several lucid review articles have been written by A. S. Wightman: Introductory remarks in *Troubles in the External Field Problem for Invariant Wave Equations* (A. S. Wightman, reviewer), Gordon and Breach, New York, 1971; "Relativistic wave equations as singular hyperbolic systems," *Proc. Symp. Pure Math.* **XXIII**, pp. 441–447, Amer. Math. Soc., 1973; "Instability phenomena in the external field problem for two classes of relativistic wave equations," in *Essays in Honor of Valentine Bargmann*, pp. 423–460, Princeton Univ. Press, Princeton, New Jersey, 1976.

There is a large literature on potential scattering for the Dirac and Klein-Gordon equations. For the Dirac equation, the reader can consult K. J. Eckhardt, "On the existence of wave operators for Dirac operators," *Manuscripta Math.* **11** (1974), 349–371; and "Scattering theory for Dirac operators," *Math. Z.* **139** (1974), 105–131; J. C. Guillot and G. Schmidt, "Spectral and scattering theory for Dirac operators," *Arch. Rational Mech. Anal.* **55** (1974), 193–206; K. Mochinzuki, "On the perturbation of the continuous spectrum of the Dirac operator," *Proc. Japan Acad.* **40** (1964), 707–712; R. Prosser, "Relativistic potential scattering," *J. Mathematical Phys.* **4** (1963), 1048–1054; M. Thompson, "Eigenfunction expansions and the associated scattering theory for potential perturbations of the Dirac equation," *Quart. J. Math. Oxford Ser.* **23** (1972), 17–55; the Veselic-Weidmann papers quoted in the Notes to Section 4; R. A. Weder, "Spectral properties of the Dirac Hamiltonian," *Ann. Soc. Sci. Bruxelles Sér. I* **87** (1973), 341–355; and O. Yamada, "On the principle of limiting absorption for the Dirac operator," *Publ. Res. Inst. Math. Sci.* **8** (1972/73), 557–577. For the Klein-Gordon theory, the references include, J. M. Chadam, "The asymptotic behavior of the Klein-Gordon equation with external potential, I, II," *J. Math. Anal. Appl.* **31** (1970), 334–348; *Pacific J. Math.* **31** (1969), 19–31; Deift's monograph quoted in the notes to Section 10; T. Kako, "Spectral and scattering theory for the j-self-adjoint operators associated with the perturbed Klein-Gordon type equations," *J. Fac. Sci. Univ. Tokyo Sect IA Math.* **23** (1976), 199–221; L. Lundberg, "Spectral and scattering theory for the Klein-Gordon equation," *Comm. Math. Phys.* **31** (1973), 243–257; M. Schechter, "The Klein-Gordon equation and scattering theory," *Ann. Physics* **101** (1976), 601–609 (see also Schechter's papers on elliptic systems quoted in the Notes to Section XIII.8 and the second

of his papers quoted in the Notes to Section 3); W. Strauss, "Scattering for hyperbolic equations," *Trans. Amer. Math. Soc.* **108** (1963), 13–37; D. Thoe, "Spectral theory for the wave equation with a potential term," *Arch. Rational Mech. Anal.* **22** (1966), 364–406; K. Veselic, "A spectral theory for the Klein-Gordon equation with an external electrostatic potential," *Nuclear Phys. A* **147** (1970), 215–224; R. Weder, "Self-adjointness and invariance of the essential spectrum for the Klein-Gordon equation," *Helv. Phys. Acta* **50** (1977), 100–117, and "Scattering theory for the Klein-Gordon equation," *J. Functional Analysis* **27** (1978).

Section XI.16 The Haag-Ruelle theory is based on work of R. Haag, "Quantum field theories with composite particles and asymptotic completeness," *Phys. Rev.* **112** (1958), 669–673; "The framework of quantum field theory," *Nuovo Cimento Supp.* **14** (1959), 131–152; and D. Ruelle, "On the asymptotic condition in quantum field theory," *Helv. Phys. Acta* **35** (1962), 147–163. Haag presented the basic elements of the proof of Theorem XI.109 including the introduction of TVEV, and he postulated the falloff of these TVEV. He did not give a rigorous proof of the falloff of regular wave packets for the Klein-Gordon equation but based his proof on the correct bounds which were only proven formally. Ruelle supplied these two details essentially by proving Theorem XI.109 by the method used in this section and the corollary to Theorem XI.17 by a related but distinct method. Earlier, various authors had obtained partial results on clustering of TVEVs: G. Dell'Antonio and P. Gulmanelli, "Asymptotic conditions in quantum field theories," *Nuovo Cimento* **12** (1959), 38–53; H. Araki, "On the asymptotic behavior of vacuum expectation values at large space like separation," *Ann. Physics* **11** (1960), 260–274; and R. Jost and K. Hepp, "Über die Matrixelemente des Translation operators," *Helv. Phys. Acta* **35** (1962), 34–46. Theorem XI.111 is due to L. Schwartz in his book on distributions (see the notes to Sections V.3 and V.4).

There are "textbook" presentations of the Haag-Ruelle theory in various places: Jost's book quoted in the notes to Section IX.8; *Introduction to Axiomatic Quantum Field Theory* by N. N. Bogoliubov, A. A. Logunov, and I. T. Todorov, Benjamin, New York, 1975; and in K. Hepp, "On the connection between Wightman and LSZ quantum field theory," pp. 135–246 in *Axiomatic Field Theory: Brandeis University, 1965* (M. Chrétien and S. Deser, eds.), Gordon and Breach, New York, 1966. All these treatments, as well as ours, follow Ruelle's approach.

If the function in Theorem XI.110 is in C_0^∞, then the falloff of $G(\alpha)$ is exponential; see H. Araki, K. Hepp, and D. Ruelle, "On the asymptotic behavior of Wightman functions in spacelike directions," *Helv. Phys. Acta* **35** (1962), 164–174.

Lorentz covariance of scattering theory is a result of Ruelle (in the paper above) and is further discussed in the above textbook presentations. Ruelle also discusses the case of higher spin particles and fields. One critical aspect of this presentation is that odd (respectively, even) spin fields only produce odd (respectively, even) spin asymptotic fields. This is critical for the physical interpretation of the spin-statistics theorem. Haag and Ruelle also discuss what to do if property 10 fails—one uses suitable polynomials in the fields. A transcription of the Haag-Ruelle theory into the C^* algebraic approach to quantum field theory appears in R. Haag and H. Araki, "Collision cross sections in terms of local observables," *Comm. Math. Phys.* **4** (1967), 77–91.

Our physical interpretation of Theorem XI.109 as a scattering theory depended on rewriting it in the form of two Hilbert space wave operators (Corollary 2), but one can also justify its interpretation by rewriting N-body nonrelativistic quantum theory as a field theory and rewriting its scattering theory in a form analogous to Theorem XI.109. This has been done in W. Sandhas, "Definition and existence of multichannel scattering states," *Comm. Math. Phys.* **3** (1966), 358–374 and in Hepp's lectures (Hepp says he is following, in part, unpublished work of W. Hunziker); see also Problem 142.

Corollary 1 of Theorem XI.109 is related to a general result proven in the C^*-algebraic approach to relativistic quantum theory; namely that $\sigma(P_\mu)$ is additive; that is, if p_μ, $q_\mu \in \sigma(P_\mu)$, then $p_\mu + q_\mu \in \sigma(P_\mu)$. This was proven by H. J. Borchers, "Local rings and the connection of spin with statistics," *Comm. Math. Phys.* **1** (1965), 281–307.

If one restricts the regular wave packets $f^{(1)}, \ldots, f^{(n)}$ to have no.ıoverlapping velocities (that is, if $p_i \in \operatorname{supp} \hat{f}^{(i)}$ and $p_j \in \operatorname{supp} \hat{f}^{(j)}$ implies that $p_i/\mu(p_i) \neq p_j/\mu(p_j)$), then $\|d\eta/dt\|$ falls off faster than t^{-N} for any N rather than only like $t^{-3/2}$. This allows one to develop a Haag–Ruelle theory in two and three space-time dimensions and also allows one to avoid Theorem XI.110; these ideas are discussed in Hepp's lectures and in his paper "On the connection between LSZ and Wightman quantum field theory," *Comm. Math. Phys.* **1** (1965), 95–111.

There is an alternative asymptotic condition which is based on proving that *matrix elements* of the relativistic field $\int A(x)f(x, s-t)\,d^3x\,ds$ approach those of φ_{in} and φ_{out} smeared as $t \to \mp\infty$ (this is to be compared with the vector convergence of Theorem XI.109). Scattering theory based on these assumptions was developed by H. Lehmann, K. Symanzik, and W. Zimmerman, "Zur Formulierung Quantisierter Feldtheorien," *Nuovo Cimento* **1** (1955), 205–225 and "The formulation of quantized field theories, II," *Nuovo Cimento* **6** (1957), 319. This "LSZ theory" is further developed in V. Glaser, H. Lehmann, and W. Zimmerman, "Field operators and retarded functions," *Nuovo Cimento* **6** (1957), 1122–1128. Hepp in the above quoted paper and lecture notes proves that, in the Haag–Ruelle framework, matrix elements of suitable smoothed fields between states $\eta^{\text{in}}(f_1, \ldots, f_n)$ where the f's have nonoverlapping velocities converge to the same matrix elements of φ_{in} as $t \to -\infty$. The first really significant result in the LSZ formalism is an explicit formula for the S-matrix in terms of the Wightman distributions. These **reduction formulas** are proven for distinct velocities in Hepp's work. The reduction formulas are the first step in the analysis of the analyticity properties of scattering amplitudes in axiomatic field theory. Certain aspects of these developments together with extensive references can be found in A. Martin, *Scattering Theory: Unitarity, Analyticity, and Crossing*, Lecture Notes in Physics **3**, Springer-Verlag, New York, Heidelberg, Berlin, 1969.

Asymptotic completeness has not yet been verified in any of the models of interacting Wightman fields that have been constructed. It can sometimes happen that asymptotic completeness fails because one has not included enough fields. An artificial example is the following: Suppose that one could construct an interacting quantum electrodynamics that did have asymptotic completeness, and then one restricted the theory to the electromagnetic field and the cyclic subspace that it generates. This theory would not be asymptotically complete because the Hilbert space would contain two-particle electron–positron states without containing the corresponding one-particle states that are not coupled to the vacuum by the electromagnetic fields since they are charged. There is strong evidence that similar phenomena will take place in certain two-dimensional self-interacting Boson fields where it is believed that certain two-particle states (soliton and antisoliton pairs) are coupled to the vacuum by the Bose field even though the corresponding single particle states are not. See, J. Fröhlich, "New super-selection sectors ("soliton-states") in two dimensional bose quantum field models," *Comm. Math. Phys.* **47** (1976), 269–310; "Phase transitions, Goldstone bosons and topological superselection rules," Part 2, *Acta Phys. Austriaca, Suppl.* **XV** (1976), 133–269; "Quantum theory of non-linear invariant wave (field) equations. Or: Super selection sectors in constructive quantum field theory," in *Invariant Wave Equations* (G. Velo and A. S. Wightman, eds.), Springer Physics Lecture Notes *73*, 1978, and J. Bellissard, J. Fröhlich, and B. Gidas, paper to appear in *Comm. Math. Phys.*

There has been considerable progress in the understanding of the weakly coupled $P(\varphi)_2$ theories in the energy region where no three-particle states occur, including a proof of "asymptotic completeness" for these energies. The basic papers are T. Spencer, "The decay of the

Bethe–Salpeter kernel in $P(\varphi)_2$ quantum field models," *Comm. Math. Phys.* **44** (1975), 143–164; T. Spencer and F. Zirilli, "Scattering states and bound states in $\lambda P(\varphi)_2$," *Comm. Math. Phys.* **49** (1975), 1–16. Further developments can be found in J. Glimm and A. Jaffe, "Two and three body equations in quantum field models," *Comm. Math. Phys.* **44** (1975), 293–320; and in J. Dimock and J.-P. Eckmann, "On the bound state in weakly coupled $\lambda(\varphi^6 - \varphi^4)_2$," *Comm. Math. Phys.* **51** (1976), 41–54; and "Spectral properties and bound state scattering for weakly coupled $\lambda P(\varphi)_2$ models," *Ann. Physics* **103** (1977), 289–314.

The TVEVs have analogues in probability theory where they are called **higher order cumulants** and in statistical mechanics where they are called **Ursell functions**. An elegant "axiomatic" characterization of Ursell functions and the resulting theory can be found in J. Percus, "Correlation inequalities for Ising spin lattices," *Comm. Math. Phys.* **40** (1975), 283–308. Among the significant results about TVEVs are an inversion formula (Problem 143), the relation to connectedness in diagrammatic expansions (Problem 144), and the following formula of P. Cartier, unpublished; see also the Percus paper quoted above and G. Sylvester, "Representations and inequalities for Ising model Ursell functions," *Comm. Math. Phys.* **42** (1975), 209–220:

$$(\psi_0, \varphi(x_1) \cdots \varphi(x_n)\psi_0)_T = \frac{1}{n}(\Psi_0, \Phi(x_1) \cdots \Phi(x_n)\Psi_0) \tag{349a}$$

$$\Phi(x_i) = \sum_{j=1}^{n} \omega^j \varphi_j(x_i) \tag{349b}$$

In (349b), ω is a primitive nth root of unity (that is, $\omega^n = 1, \omega^j \neq 1, j = 1, \ldots, n-1$) and $\varphi_1, \ldots, \varphi_n$ are independent copies of φ; that is, we take $\mathscr{H}' = \mathscr{H} \otimes \cdots \otimes \mathscr{H}$ (n times), $\Psi_0 = \psi_0 \otimes \cdots \otimes \psi_0$ and

$$\varphi_j(x) = 1 \otimes \cdots \otimes \varphi(x) \otimes \cdots \otimes 1 \qquad (j\text{th place})$$

Scattering theory for massless particles in an axiomatic (C^*-algebraic) framework has been developed in two remarkable papers by D. Buchholz, "Collision theory for massless fermions," *Comm. Math. Phys.* **42** (1975), 269–279; and "Collision theory for massless bosons," *Comm. Math. Phys.* **52** (1977), 147–173. While Buchholz uses some parts of the Haag–Ruelle theory, temperedness of the TVEV does not hold, so very different ideas are needed. In fact, the key idea is to exploit the fact that solutions of the wave equation obey Huygens' principle. For this reason, once the limit of $A_f(t)\Omega_0$ (suitably defined) is controlled (this is not independent of time because one cannot separate the one-particle zero mass states from the continuum), one can control the limit of $A_f(t)F\Omega_0$ for any F obtained by smearing fields with functions supported in suitable sets (basically the "hole" obtained by excluding the union of the boundaries of the light cones with vertex at points in $\operatorname{supp} f(x, t=0)$). In this way one obtains the existence of $\lim A_f(t)\psi$ for a dense set of ψ.

It is to be emphasized that when massless particles are present, one does not know how to construct scattering states for the *massive* particles. In fact, it is not clear how to "separate" the massive particle from the massless ones—it may be that in a theory of electrons and photons there is no discrete piece of the mass spectrum corresponding to one electron but that somehow only electrons accompanied by infinitely many low energy photons occur—this problem which is not completely understood, is called the **infrared problem**. There is an exhaustive literature on this subject beginning with F. Bloch and A. Nordsieck, "A note on the radiation field of the electron," *Phys. Rev.* **52** (1937), 54–59; and D. Yennie, S. Frautschi, and H. Suura, "The infrared divergence phenomena and high-energy processes," *Ann. Physics* **13** (1961), 379–452. For a discussion of more recent literature, see J. Fröhlich, "On the infrared problem in a model of

scalar electrons and massless, scalar bosons," *Ann. Inst. H. Poincaré Sect. A* **19** (1973), 1–103. It should also be mentioned that this same phenomenon could occur with the massless particles, in which case Buchholz's theory would not apply since he assumes that states with $H^2 - \mathbf{P}^2 = 0$ $(H \neq 0)$ occur.

Section XI.17 The discussion in this section is based primarily on the beautiful paper of V. Enss, "Asymptotic completeness for quantum mechanical potential scattering," *Comm. Math. Phys.*, to appear. We use some technical devices borrowed from B. Simon, "Phase space analysis of simple scattering systems: Extensions of some work of V. Enss," *Duke Math. J.*, to appear. This latter paper extends the theory to allow H_0 to be replaced by a wide variety of differential and pseudo-differential operators including Dirac Hamiltonians. Enss has extended the method to include Coulomb potentials and has presented a program, which he is currently implementing, to handle multiparticle scattering.

Wiener's theorem (Theorem XI.114) was proven by N. Wiener in his book *The Fourier Integral and Certain of Its Applications*, Cambridge University Press, London, 1935. Its consequences (including the corollary to Theorem XI.115) have been used in ergodic theory for many years; see especially, Section 8 of K. Jacobs, *Lecture Notes on Ergodic Theory*, Aarhus Lecture Note Series **1** (1962/63).

The importance of Wiener's theorem for geometrically characterizing the continuous spectrum in scattering problems was discovered independently by Lax–Phillips–de Leeuw (see p. 145 in the book of Lax and Phillips quoted in the notes to Section 11) and by D. Ruelle, "A remark on bound states in potential scattering theory," *Nuovo Cimento A* **61** (1969), 655–662. Lax–Phillips use Wiener's theorem to prove directly the corollary to Theorem XI.115 and they then use that to establish (219). Ruelle proved for a large class of Schrödinger operators including multiparticle ones that, for all R,

$$\frac{1}{2T}\int_{-T}^{T} \|F(|x| \leq R)e^{-itH}\varphi\|^2\, dt \to 0$$

as $T \to \infty$ if and only if $\varphi \in P_{\text{cont}}(H)$. W. Amrein and V. Georgescu in "Bound states and scattering states in quantum mechanics," *Helv. Phys. Acta* **46** (1973), 633–658, extended Ruelle's results and, in particular, realized that the compactness of $F(|x| \leq R)(H+i)^{-1}$ was the critical factor (this was disguised in Ruelle's discussion). None of these authors noted the uniformity in φ (one can use Wiener's theorem directly to show that $(\psi, e^{-itA}\varphi)$ goes to zero in L^2 mean if ψ is in $\mathscr{H}_{\text{cont}}$); the stated uniformity is an unpublished remark of Enss.

The final theorem in the appendix is due to V. Enss.

NOTES ON SCATTERING THEORY ON C^*-ALGEBRAS

There is a simple generalization of scattering theory ideas to the framework of C^*-algebras. In these notes we shall discuss some of the more interesting aspects of these ideas using freely the terminology of C^*-algebras. This discussion should be supplemented with the explicit examples to be found in the references below.

First, we want to discuss the relation of scattering theory to the approach to equilibrium in statistical mechanics. As a starting point, let H_0 be a self-adjoint operator on a Hilbert space $\mathscr{H}$

and let V be in $\mathscr{L}(\mathscr{H})$. Consider the natural automorphisms on $\mathscr{L}(\mathscr{H})$: $\alpha_t^{(0)}(A) = e^{iH_0t}Ae^{-iH_0t}$ and $\alpha_t(A) = e^{iHt}Ae^{-iHt}$ where $H = H_0 + V$. Let $\beta_t = \alpha_t\alpha_{-t}^{(0)}$. Then

$$\frac{d}{dt}\beta_t(A) = i\beta_t(\alpha_t^{(0)}[V, \alpha_{-t}^{(0)}(A)]) = i\beta_t([\alpha_t^{(0)}(V), A])$$

or

$$\beta_t(A) = A + i\int_0^t \beta_s([\alpha_s^{(0)}(V), A])\, ds \tag{350}$$

(350) can be solved by iteration:

$$\beta_t(A) = A + \sum_{n=1}^{\infty} \beta_t^{(n)}(A) \tag{351}$$

with

$$\beta_t^{(n)}(A) = (i)^n \int_0^t \int_0^{s_1} \int_0^{s_2} \cdots \int_0^{s_{n-1}} [\alpha_{s_n}^{(0)}(V), [\alpha_{s_{n-1}}^{(0)}(V), \ldots [\alpha_{s_1}^{(0)}(V), A] \cdots]]\, ds_n\, ds_{n-1} \cdots$$

A simple estimate shows that $\|\beta_t^{(n)}(A)\| \leq 2^n(t^n/n!)\|V\|^n\|A\|$, so the series (351) converges to a solution of (350). Equivalently:

$$\alpha_t(A) = \alpha_t^{(0)}(A) + \sum_{n=1}^{\infty} (i)^n \int_{0 \leq s_n \leq \cdots \leq s_1 \leq t} [\alpha_{s_n}^{(0)}(V), [\cdots, [\alpha_{s_1}^{(0)}(V), \alpha_t^{(0)}(A)] \cdots]\, ds_1 \cdots ds_n \tag{352}$$

(352), which expresses α_t in terms of only $\alpha_t^{(0)}$ and V, is the starting point for a general theory of perturbations of automorphisms of C^*-algebras. For suppose that $\alpha_t^{(0)}$ is a norm-continuous one-parameter group of automorphisms of a C^*-algebra $\mathfrak{A}$ and let $V \in \mathfrak{A}$. The expression in (352) converges to a norm-continuous one-parameter group of automorphisms which we denote by α_t. It is now fairly easy to prove (see Problem 147):

Theorem XI.117 Let π be a representation of a C^*-algebra $\mathfrak{A}$ on a Hilbert space $\mathscr{H}$ and let $\alpha_t^{(0)}$ and α_t be as above. Suppose that there is a one-parameter strongly continuous unitary group U_t on $\mathscr{H}$ with

$$\pi(\alpha_t^{(0)}(A)) = U_t\pi(A)U_{-t} \tag{353a}$$

Let H_0 be the infinitesimal generator of U_t and let $W_t = e^{i(H_0 + \pi(V))t}$. Then

$$\pi(\alpha_t(A)) = W_t\pi(A)W_{-t} \tag{353b}$$

Conversely, if (353b) holds for some W_t, then (353a) holds for some U_t.

Thus, we see that $\alpha_t^{(0)}$ and α_t are unitarily implementable in precisely the same representations.

Now one seeks to control $\lim_{t \to \mp\infty} \alpha_{-t}\alpha_t^{(0)}(A)$. (352) and Cook's method (Section 3) immediately imply:

Theorem XI.118 Suppose that for a dense subspace $\mathfrak{A}_0 \subset \mathfrak{A}$ and all $A \in \mathfrak{A}_0$,

$$\|[\alpha_{(\cdot)}^{(0)}(V), A]\| \in L^1(\cdot) \tag{354}$$

Then for any $A \in \mathfrak{A}$, $\lim_{t \to \pm\infty} \alpha_{-t}\alpha_t^{(0)}(A)$ exist and $w^{\pm} = \text{s-lim}_{t \to \mp\infty} \alpha_{-t}\alpha_t^{(0)}$ are injective morphisms on $\mathfrak{A}$ obeying

$$w^{\pm}(\alpha_s^{(0)}(A)) = \alpha_s(w^{\pm}(A)) \tag{355}$$

D. Robinson has suggested a very beautiful connection between Theorem XI.118 and the approach to equilibrium in quantum lattice gases: Let $\alpha_t^{(0)}$ be the time translations in a lattice gas. Let V be a local observable. Then, if A is a local observable, (354) is to be expected (and can be proven in some models!) since as $t \to \pm\infty$, $\alpha_t^{(0)}(V)$ is "spread out" over a larger and larger region. Let φ be an invariant state for α_t, that is, for the locally perturbed dynamics. Then $\varphi(\alpha_t^{(0)}(\cdot)) = \varphi(\alpha_{-t}\alpha_t^{(0)}(\cdot)) \to \varphi(w^{\pm}(\cdot))$ and, by (355), $\varphi(w^{\pm}(\cdot))$ are invariant states for $\alpha_t^{(0)}$. Thus, if φ moves according to the free dynamics, it approaches an invariant state for $\alpha_t^{(0)}$. Moreover, under some additional hypotheses, if φ is a KMS state for α_t at temperature T, then $\varphi(w^{\pm}(\cdot))$ are KMS states for $\alpha_t^{(0)}$ at temperature T.

This example of C^*-algebra scattering theory and its relation to statistical mechanics is due to D. Robinson, "Return to equilibrium," *Comm. Math. Phys.* **31** (1973), 171–189. Robinson's paper contains the details of the theorems discussed above and calculations in some explicit models. Some aspects of the C^*-algebra approach to scattering used by Robinson already appeared in R. F. Streater, "On certain non-relativistic quantized fields," *Comm. Math. Phys.* **7** (1968), 93–98; and K. Hepp, "Rigorous results on the s-d model of the Kondo effect," *Solid State Comm.* **8** (1970), 2087–2090. For additional discussion of approach to equilibrium in statistical mechanics (from a nonscattering point of view), see C. Radin, "Gentle perturbations," *Comm. Math. Phys.* **23** (1971), 189–198; O. Lanford, III and D. Robinson, "Approach to equilibrium of free quantum systems," *Comm. Math. Phys.* **24** (1972), 193–210.

In many cases (354) is too strong and $\alpha_{-t}\alpha_t^{(0)}$ is not norm convergent but only weakly convergent. In such cases it is more natural to suppose that $\mathfrak{A}$ is a von Neumann algebra. An approach of this sort is used in some studies of long-range potential scattering. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$. Let $\mathfrak{A} = \{H_0\}'$, the family of operators commuting with bounded functions of H_0. Let V be a long-range potential of the sort for which modified wave operators exist. Let $\alpha_t(A) = e^{iHt}Ae^{-iHt}$ (which may not be in $\mathfrak{A}$ but only in $\mathscr{L}(\mathscr{H})$). Then

$$\underset{t\to\mp\infty}{\text{w-lim}}\ \alpha_t(A) = \underset{t\to\mp\infty}{\text{w-lim}}\ e^{iHt}U_D(-t)AU_D(t)e^{-iHt} = \Omega_D^{\pm}A(\Omega_D^{\pm})^*$$

References for the C^*-algebra approach to long-range scattering can be found in the notes to Section 9.

Scattering in terms of automorphisms also plays a role in the study of spectral properties of Hamiltonians in certain cutoff quantum field theory models. Let us indicate the general ideas in the application to the cutoff $P(\varphi)_2$ field theory. Let $a_t^*(f) = e^{iHt}e^{-iH_0t}a^*(f)e^{iH_0t}e^{-iHt}$. Formally,

$$\frac{d}{dt}a_t^*(f) = ie^{iHt}[V, e^{-iH_0t}a^*(f)e^{iH_0t}]e^{-iHt}$$

This formula, the Cook method, and certain estimates of L. Rosen, "The $(\varphi^{2n})_2$ quantum field theory: Higher order estimates," *Comm. Pure Appl. Math.* **24** (1971), 417–457, allow one to prove that $\lim_{t\to\mp\infty} a_t^*(f)\psi$ exist for a family of f's dense in the one-particle space and ψ's dense in Fock space. The limiting operators $a_{\pm}^*(f)$ can be shown to have three important additional properties: (1) $[a_{\pm}^*(f), a_{\pm}(g)] = -(Cf, g)$; enough control on the limit allows one to prove that the algebraic relations are preserved. (2) Since e^{iH_0t} is of the special form $e^{iH_0t} = \Gamma(e^{i\omega t})$ for a one-particle operator ω, the intertwining relations take the form $e^{iHt}a_{\pm}^*(f)e^{-iHt} = a_{\pm}^*(e^{i\omega t}f)$. (3) If ψ is an eigenvector of H, then $a_{\pm}(f)\psi = 0$ for all f. This follows from the fact that $\text{s-lim}_{t\to\pm\infty} a(e^{i\omega t}f)N^{-1/2} = 0$ and Rosen's estimates. (1) and (3) allow one to build up a subspace $\mathscr{H}_\psi \subset \mathscr{H}$ and a Fock representation for $a_{\pm}^*(f)$ with ψ as vacuum for any eigenvector ψ of H. Since it is known that there is a vector with $H\psi = E_0\psi$ (see Section XIII.12), (2) and this construction imply that $H \restriction \mathscr{H}_\psi$ is unitarily equivalent to $H_0 + E_0$ from which it follows that $[m_0 + E_0, \infty) \subset \sigma_{ac}(H)$.

The idea of using scattering theory to study quantum field Hamiltonians via the construction of asymptotic creation and annihilation operators $a_{\pm}^*$ was first presented in Y. Kato and N. Mugibayashi, "Regular perturbations and asymptotic limits of operators in quantum field theory," *Progr. Theoret. Phys.* **30** (1963), 103–133; and developed in a series of papers by R. Höegh-Krohn, "Asymptotic limits in some models of quantum field theory, I, II, III," *J. Mathematical Phys.* **9** (1968), 2075–2080; **10** (1969), 639–643; **11** (1970), 185–188; and "On the scattering operator for quantum fields," *Comm. Math. Phys.* **18** (1970), 109–126. The theory was used to study spectral properties of spatially cutoff $P(\varphi)_2$ Hamiltonians (see Sections X.7 and X.9) by R. Höegh-Krohn, "On the spectrum of the space cutoff $:P(\varphi):$ Hamiltonian in two space-time dimensions," *Comm. Math. Phys.* **21** (1971), 256–260; and Y. Kato and N. Mugibayashi, "Asymptotic fields in the $\lambda(\varphi^4)_2$ quantum field theory," *Progr. Theoret. Phys.* **45** (1971), 628–639; and for the Y_2 field theory by J. Dimock, "Spectrum of local Hamiltonians in the Yukawa$_2$ field theory," *J. Mathematical Phys.* **13** (1972), 477–481. In either case, one proves that $[m_0 + E_0, \infty) \subset \sigma_{ac}(H)$ where $E_0 = \inf \sigma(H)$ and m_0 is the free mass in H_0. Since one knows that $\sigma_{ess}(H) \subset [m_0 + E_0, \infty)$ by results of J. Glimm and A. Jaffe, "The $\lambda(\varphi^4)_2$ quantum field theory without cutoffs, II: The field operators and the approximate vacuum," *Ann. of Math.* **91** (1970), 362–401, (for $(\varphi^4)_2$) and "Self-adjointness of the Yukawa$_2$ Hamiltonian," *Ann. Physics* **60** (1970), 321–383 (for Y_2); and of L. Rosen "A $\lambda\varphi^{2n}$ field theory with cutoffs," *Comm. Math. Phys.* **16** (1970), 157–183 (for $P(\varphi)_2$); one can conclude that $\sigma_{ac}(H) = \sigma_{ess}(H) = [m_0 + E_0, \infty)$ for these models. We remark that the methods of Kato-Mugibayashi and Höegh-Krohn are restricted to models for which there is no renormalization of Hilbert space. For realistic field theories, one must fall back on the Haag-Ruelle theory of Section 16.

PROBLEMS

†1. Under hypotheses (3), prove that for any $\langle r_0, v_0\rangle \in \mathbb{R}^6$, there is a solution of (2) for all time. (*Hint:* Consult the discussion of classical motion on the real line in the appendix to Section X.1.)

2. Prove that if (4a) holds, but not necessarily (4b), then the map constructed in the proof of Theorem XI.1 has at least one fixed point.

3. Find an example of a force F for which (4a) holds, where (4b) is false, and where the map in Theorem XI.1 has more than one fixed point, that is, where scattering states exist but are not unique.

Reference for Problems 2, 3: The paper of Simon quoted in the notes to Section XI.2.

†4. Prove that under the hypothesis that F obeys (4), the integral equation (6) is equivalent to the differential equation (2a) with boundary conditions (5).

†5. Let $\mathscr{M}$ be a complete metric space and let $c < 1$.
   (a) Let $\{F_n\}$, F_∞ be a family of maps on M obeying $\rho(F_n x, F_n y) \le c\rho(x, y)$ for all n and all $x, y \in \mathscr{M}$. Suppose that $F_\infty x = \lim_{n\to\infty} F_n x$ for all x and that $F_n x_n = x_n$, $F_\infty x_\infty = x_\infty$. Prove that $x_n \to x_\infty$.
   (b) Let F: $\mathbb{R} \times \mathscr{M} \to \mathscr{M}$ be continuous and obey $\rho(F(t, x), F(t, y)) \le c\rho(x, y)$ where $c < 1$. Suppose that $\mathscr{M}$ is a subset of a Banach space and that $F(t, x)$ is C^∞ jointly

in x and t as a map from $\mathbb{R} \times \mathcal{M}$ into $\mathcal{M}$ (differentiable in the Fréchet sense). Define $g(t) \in \mathcal{M}$ by $F(t, g(t)) = g(t)$. Prove that $g(t)$ is a C^∞ vector-valued function.

†6. Complete the proof of Theorem XI.2a.

†7. Prove that under the hypotheses of Theorem XI.2, the map $\mathcal{F}_{a,b}^{(-\infty)}: \Sigma_0 \times \mathcal{M}_T \to \mathcal{M}_T$ obeys all the hypotheses of Problem 5b with the obvious modification necessary when $\mathbb{R}$ is replaced by a subset of $\mathbb{R}^6$.

*8. Develop scattering theory in n-body classical systems in the scattering channel where all particles are asymptotically free. Consider the problems that arise in attempting the extension to channels with some bound states.

9. Find a central force and a solution of Newton's equation in that force field for which $\lim_{t\to-\infty} |r(t)| = \infty$; $\lim_{t\to+\infty} |r(t)| = r_0 < \infty$.

†10. Prove that the sets Σ_{bound}, Σ_0, $N_\pm$, $N_\pm^{(n)}$, Σ' used in the proof of Theorem XII.3 are all measurable.

11. Prove formulas (7a) and (7b) for the functions $\theta(E, \ell)$ and $T(E, \ell)$ in a central force field. *Reference:* Newton's book quoted in the notes to Section 2.

12. Verify the formula for $d\sigma/d\Omega$ in the central case.

13. Consider the statement: Total cross sections are usually infinite in classical mechanics.

14. In the context of Theorem XI.3 but with the additional hypothesis that $V(\mathbf{r})$ is a central potential, find an alternative proof that if $E > 0$ and $\overline{\lim}_{t\to\infty} |r(t)| = \infty$, then $\lim_{t\to\infty} |r(t)|t^{-1} > 0$. (*Hint:* Use conservation of energy and angular momentum.)

15. (a) Let A be a self-adjoint operator. Prove that $e^{i(A-\lambda)t}\varphi$ has a norm limit as $t \to \infty$ if and only if φ is an eigenvector of A with eigenvalue λ. (*Hint:* Compute the weak limit of $T^{-1}\int_0^T e^{i(A-\lambda)t}\varphi\, dt$.)
(b) Let A and B be self-adjoint. Prove that $e^{iAt}e^{-iBt}$ converges in operator norm as $t \to \pm\infty$ if and only if $A = B$.

16. Let H_0 be a fixed operator and let V_n and V_∞ be H_0-bounded operators with relative bound a less than 1, so that $H_0 + V_n \to H_0 + V_\infty$ in strong resolvent sense. Suppose that there is a dense set, D in $P_{ac}(H_0)$ so that for $u \in D$: $\sup_{n\le\infty} \|V_n e^{-itH_0}u\| \equiv f_u(t)$ is in $L^1(\mathbb{R})$. Prove that $\Omega^\pm(H_0 + V_n, H_0)$ converge strongly to $\Omega^\pm(H_0 + V, H_0)$. (*Hint:* First show that $\Omega(H_0 + V_n, H_0)u = u + i\int_0^\infty e^{i(H_0+V_n)t}V_n e^{-itH_0}u$ and then use dominated convergence.) *Reference:* The paper of Davies quoted in the notes to Section 4.

†17. (a) Show that $|||\cdot|||$ is a norm on $\mathcal{M}(B)$. Is $\mathcal{M}(B)$ complete in this norm? (*Hint:* Use (16).)
(b) Show that $\mathcal{M}(B)$ is dense in $P_{ac}(B)$ in the usual norm.

18. Let C be a bounded operator with $C(A + i)^{-n}$ compact for some n where A is self-adjoint. Prove that $Ce^{-iAt}P_{ac}(A) \to 0$ strongly as $t \to \pm\infty$. Prove the same thing if $CE_I(A)$ is compact for all bounded intervals I.

19. Prove Theorem XI.5 by first showing that s-lim $e^{iAt}(1 - \chi)e^{-iBt}$ exist and then, using Problem 18, that s-lim $\chi e^{-iBt} = 0$.

20. Let A and B be self-adjoint operators with $Q(A) = Q(B)$. Let $\varphi, \psi \in Q(A)$. Prove that $(\varphi, e^{iAt}e^{-iBt}\psi)$ is differentiable with derivative $i(\varphi, e^{iAt}(A - B)e^{-iBt}\psi)$ and verify (15).

†21. Fill in the domain details in the proof of Pearson's theorem (Theorem XI.7).

22. Construct operators A_n and A so that $\|A_n - A\|_1 \to 0$, so that A_n has purely absolutely continuous spectrum $[0, 1]$, and so that A has absolutely continuous spectrum $[0, 1]$ and an eigenvalue at $\lambda = 0$. Conclude that $\Omega^\pm(A, A_n)$ cannot converge strongly to $\Omega^\pm(A, A)$.

23. Let $(A_n + i)^{-1} \to (A + i)^{-1}$ in trace class norm. Let $J_n = (A_n + i)^{-1}(A + i)^{-1}$ and $J = (A + i)^{-2}$. Prove that $\Omega^\pm(A_n, A; J_n) \to \Omega^\pm(A, A; J)$ strongly and conclude that $\Omega^\pm(A_n, A) \to P_{ac}(A)$. *Hint:* Use the fact that

$$\Omega^\pm(A_n, A; J_n)(A + i)^2 = \Omega^\pm(A_n, A)$$

Prove that $\Omega^\pm(A, A_n)P_{ac}(A) \to P_{ac}(A)$ strongly.

24. Suppose that $E_I(A_n)(A_n - A)E_I(A)$ goes to zero in trace class norm for each bounded interval I. Suppose, moreover, that the A_n are uniformly subordinate to A, that is, the functions involved in the definition of subordinate can be chosen to be independent of n. Prove that $\Omega^\pm(A_n, A) \to P_{ac}(A)$ and $\Omega^\pm(A, A_n)P_{ac}(A) \to P_{ac}(A)$ strongly.

25. Suppose that A and B are self-adjoint operators with $(A - z)^{-n} - (B - z)^{-n}$ trace class for all Im $z \neq 0$.
(a) Prove that $(A + i)^{-k} - (B + i)^{-k}$ is compact for any integer $k > n$. (*Hint:* Take derivatives by using the Cauchy integral formula.)
(b) Let $J = \sum_{j=1}^n (A + i)^{-j}(B + i)^{-n+j-1}$. Use Pearson's theorem to prove that $\Omega^\pm(A, B; J)$ exist.
(c) Let $J' = (A + i)^{-n+1}J$. Prove that $\Omega^\pm(A, B; J')$ exist.
(d) Let $J'' = (B + i)^{-2n}$. Prove that $\Omega^\pm(A, B; J'')$ exist and equal $n\Omega^\pm(A, B; J')$. (*Hint:* Use (a).)
(e) Prove that $\Omega^\pm(A, B)$ exist and are complete.

†26. Prove part (a) of Lemma 3 used in the Kato–Birman theory.

27. Let A and B be self-adjoint operators. Prove that $(A - z)^{-1} - (B - z)^{-1}$ is trace class for some $z \in \rho(A) \cap \rho(B)$ if and only if it is trace class for all $z \in \rho(A) \cap \rho(B)$.

28. Let $A_n \to A$ in trace class norm. Let φ be an admissible function. Prove that $\Omega^\pm(\varphi(A_n), \varphi(A)) \to P_{ac}(A)$ and $\Omega^\pm(\varphi(A), \varphi(A_n))P_{ac}(A) \to P_{ac}(A)$ strongly as $n \to \infty$.

29. (a) Let $F(z) = (A + E)^{-z-\frac{1}{2}}C(B + E)^{-k(1-z)-\frac{1}{2}}$. Suppose that $F(0)$ and $F(1)$ are trace class. Prove that $F(z)$ is trace class for all z with $0 \le \text{Re } z \le 1$. (*Hint:* Apply the three lines lemma to $\text{Tr}(F(z)K)$ for finite rank K.)
(b) Prove (36).

30. Prove Proposition 5 of Section 3.

31. (a) Let $A = -d^2/dx^2$ on $L^2(0, \infty)$ with $u(0) = 0$ boundary conditions. Let $B = A + V$ defined as a sum of quadratic forms where $V \in L^1_{\text{loc}}(0, \infty)$ is positive (V may have arbitrarily bad growth at $r = 0$) and supp $V \subset [0, 1]$. Let $\tilde{A} = -d^2/dx^2$ on $L^2(0, 1) \oplus L^2(1, \infty)$ with $u(0) = u(1) = 0$ boundary conditions on the first factor and $u(1) = 0$ boundary conditions on the second. Let $\tilde{B} = \tilde{A} + V$. Prove that $(\tilde{A} + 1)^{-1} - (A + 1)^{-1}$ and $(\tilde{B} + 1)^{-1} - (B + 1)^{-1}$ are trace class (*Hint:* They are finite rank.)

(b) Let $\tilde{A} = A_1 \oplus A_2$. Prove that $(A_1 + 1)^{-1}$ and $(B_1 + 1)^{-1}$ are trace class and conclude that $(\tilde{A} + 1)^{-1} - (\tilde{B} + 1)^{-1}$ is trace class.
(c) Prove that $(A + 1)^{-1} - (B + 1)^{-1}$ is trace class.
*(d) Extend these ideas to n dimensions. (*Hint:* See the paper of Deift and Simon quoted in the notes to Section 4.)

32. (a) Given an operator A on a Hilbert space $\mathscr{H}$ that is not densely defined but with A self-adjoint on $D(A)$, define e^{iAt} and $(A + i)^{-1}$ on $\mathscr{H}$ by setting them to zero on $D(A)^{\perp}$. Extend the Kuroda-Birman theorem to this setting.
(b) Let $B = -\Delta$ on $L^2(\mathbb{R}^n)$ and A be the operator on $L^2(\mathbb{R}^n \backslash \{x \mid |x| < 1\})$ with Dirichlet boundary conditions on the sphere. Prove that the Kuroda-Birman theorem in the extended form (a), with $(A + i)^{-n}$ replacing $(A + i)^{-1}$, is applicable. Is Birman's theorem applicable?
(c) Use these ideas to discuss obstacle scattering (Section 10) without the trick of adding dynamics to the interior.

*†33. (a) Prove Theorem XI.19a by using finite propagation speed.
(b) Let $\varphi(x, t)$ solve the wave equation with initial data in $\mathscr{S}(\mathbb{R}^n)$. Let $x = \langle x_1, 0, \ldots, 0 \rangle$ with $x_1 > 0$. Prove that $\varphi(x, t) = \varphi_+(x, t) + \varphi_-(x, t)$ with

$$\varphi_{\pm}(x, t) = \int_{S^{n-1}} d\Omega \int_0^{\infty} \alpha^{n-2} e^{i\alpha(\pm t + x_1 \cos\theta)} f_{\pm}(\alpha, \Omega)\, d\alpha$$

with $f_{\pm}$ smooth on $(0, \infty) \times S^{n-1}$ and continuous up to $\alpha = 0$.
(c) Prove that

$$\varphi_{\pm}(x, t) = \int_{S^{n-1}} g_{\pm}(\pm t + x_1 \cos\theta, \Omega)\, d\Omega$$

where $|g_{\pm}(y, \Omega)| \leq C(1 + |y|)^{-(n-1)}$ and conclude that Theorem XI.19b holds.
(d) Make a stationary phase analysis in the $d\Omega$ variables to analyze the behavior if $|x|/t \in (1 - \varepsilon, 1 + \varepsilon)$ and complete the proof of Theorem XI.19c.

34. Apply stationary phase methods to time-dependent scattering theory.

†35. Fill in the details of the interpolation argument needed in the proof of Theorem XI.20.

36. Let $f(y) = e^{-y^2}$. Suppose that g is not in $L^2_{\text{loc}}(\mathbb{R}^n)$. Prove that $g(x)f(-i\nabla)$ is *not* a bounded operator and conclude that Theorem XI.20 does not extend to L^q for $q < 2$.

37. Let $\|f\|_{BS} = \sum_{m \in \mathbb{Z}^n} (\int_{0 \leq x_i - m_i < 1} |f(x)|^2\, dx)^{1/2}$. Prove that if f and g satisfy $\|f\|_{BS} + \|g\|_{BS} < \infty$, then $f(x)g(i\nabla)$ is trace class and

$$\|f(x)g(-i\nabla)\|_1 \leq c\|f\|_{BS}\|g\|_{BS}$$

(*Hint:* Use Theorem XI.21 to prove that $\|f(x)g(i\nabla)\|_1 \leq c\|f\|_2\|g\|_2$ for any f and g each with support in some unit cube.)

Remark: The $\|\cdot\|_{BS}$ norm was used by Birman and Solomjak in their paper quoted in the notes to Section 3.

38. Suppose that $(1 + x^2)^{\delta/2} f(x)$ and $(1 + x^2)^{\delta/2} g(x)$ lie in $L^p(\mathbb{R}^n)$ where $2 \leq p < \infty$ and $\delta > n/p$. Prove that $f(x)g(-i\nabla)$ is in $\mathscr{I}_{p/2}$. (*Hint:* Interpolate from Theorem XI.21.)

39. Suppose that $\Omega^{\pm}(A, B)$ exist.
(a) Prove that $(1 - P_{[a,b]}(A))\Omega^{\pm}(A, B)P_{[a,b]}(B) = 0$.
(b) Let $\varphi(x) = \alpha x + \beta$ for $x \in [a, b]$. Prove that:

$$\Omega^{\pm}(\varphi(A), \varphi(B))P_{[a,b]}(B) = \begin{cases} \Omega^{\pm}(A, B)P_{[a,b]}(B), & \alpha > 0 \\ \Omega^{\mp}(A, B)P_{[a,b]}(B), & \alpha < 0 \end{cases}$$

(c) Prove an invariance principle for piecewise linear φ.

40. Under the coordinate change $R = (\mu_1 + \mu_2)^{-1}(\mu_1 r_1 + \mu_2 r_2)$, $r = r_2 - r_1$, show that $H = -(2\mu_1)^{-1}\Delta_1 - (2\mu_2)^{-1}\Delta_2 + V(r_1 - r_2)$ becomes

$$H = -(2M)^{-1}\Delta_R - (2m)^{-1}\Delta_r + V(r)$$

in the passive interpretation where $M = \mu_1 + \mu_2$ and $m^{-1} = \mu_1^{-1} + \mu_2^{-1}$.

41. Suppose that S is an $N \times N$ matrix and consider the coordinate change $x_i = \sum s_{ij} y_j$ on $\mathbb{R}^{3N}$. Suppose that $\sum_{i=1}^N (2\mu_i)^{-1}\Delta_{x_i}$ is transformed to $\sum_{i=1}^N (2\mu_i)^{-1}\Delta_{y_i}$ and that for all i and j, $x_i - x_j = \sum_{k=1}^{N-1} a_{ijk} y_k$ (note the $N - 1$). Prove that $y_N = a \sum_{i=1}^N \mu_i x_i$ where $a = (\sum_{i=1}^N \mu_i)^{-1/2} \mu_N^{-1/2}$.

†42. Prove (56) from (55).

†43. Prove that the linear combinations of the translates of $\varphi_\gamma(x) = \gamma^{-\frac{1}{4}} e^{-\frac{1}{2}\gamma x^2}$ are dense in $L^2(\mathbb{R}^3)$. (*Hint:* Obtain Hermite functions by taking derivatives.)

44. Suppose that $\int (1 + |y|)^{\alpha} |V(y)|^2\, d^n y < \infty$ for some α with $n + \alpha > 2$. Prove that (45) holds, and conclude that $\Omega^{\pm}(-\Delta + V, -\Delta)$ exist. *Remark:* This result, unlike Theorem XI.24, holds in the case $n = 1, 2$.

45. Suppose that $V_t(x)$ is a family of functions with support in a fixed compact region whose L^2 norms are bounded by some power of t. Use stationary phase methods to prove that the time-dependent wave operators exist.

46. Suppose that A is a positive self-adjoint operator and B is a self-adjoint operator with:
(i) $|B|$ is A-form bounded with relative bound $\alpha < 1$.
(ii) $|B|^{1/2}(A + i)^{-1}$ is trace class.
Prove that $(A + B + E)^{-1} - (A + E)^{-1}$ is trace class for E sufficiently large. (*Hint:* Let $B^{1/2} = B/|B|^{1/2}$ and use the formula

$$(A + B + E)^{-1} - (A + E)^{-1} = -(A + E)^{-1}B^{1/2}(1 + |B|^{1/2}(A + E)^{-1}B^{1/2})^{-1}|B|^{1/2}(A + E)^{-1}.)$$

47. (a) Prove that the kernel of $[-d^2/dx^2 + 1]^{-1}$ on $L^2(\mathbb{R})$ is $\frac{1}{2}e^{-|x-y|}$. (*Hint:* Use the Fourier transform.)
(b) Let h_0 be the operator $-d^2/dx^2$ on $L^2(0, \infty)$ with zero boundary conditions at the origin. Prove that the kernel of $(h_0 + 1)^{-1}$ is $\frac{1}{2}e^{-|x-y|} - \frac{1}{2}e^{-|x+y|} = K(x, y)$. (*Hint:* Prove that $\int K(x, y)f(y)\, dy$ is in $D(h_0)$ and that $h_0 + 1$ applied to it is f.)

48. (a) Let V be in L^2 with compact support. Knowing (63) for continuous V_n, prove it for V.
(b) For arbitrary V, let V_n be in L^2 with compact support and $V_n \uparrow |V|$ pointwise. Prove (63) for V.

†49. Prove the proposition preceding Theorem XI.33 concerning properties of the S-operator in two-body systems.

50. Let A be a positive self-adjoint operator and let B_∞ and B_n be self-adjoint operators, so that:

(i) $|B_n| \leq \frac{1}{2}A + c$ for some fixed c and all n.
(ii) $|B_n|^{1/2}(A+i)^{-1} \to |B_\infty|^{1/2}(A+i)^{-1}$ in Hilbert-Schmidt norm.
(iii) $[B_n/|B_n|^{1/2}](A+i)^{-1} \to [B_\infty/|B_\infty|^{1/2}](A+i)^{-1}$ in Hilbert-Schmidt norm.

Prove that $(A + B_n + i)^{-1} \to (A + B_\infty + i)^{-1}$ in trace norm.

51. The Klein-Gordon equation restricted to positive frequencies is a Schrödinger type equation $i\psi_t = H\psi$ with $H = \sqrt{-\Delta + V(x) + m_0^2}$ where V is such that $-\Delta + V \geq -m_0^2$. Let $H_0 = \sqrt{-\Delta + m_0^2}$. Prove that:
(a) If $V \in L^{3/2} + L^\infty$ and H is the square root of the operator defined as a form sum, then $C_0^\infty(\mathbb{R}^3)$ is an operator core for H.
(b) If $V \in L^1 \cap L^{3/2}$, then the wave operators $\Omega^\pm = \text{s-lim}_{t \to \mp\infty} e^{itH}e^{-itH_0}$ exist and are complete. (*Hint:* Use the invariance principle.)

†52. (a) Verify the form of H_0 under change to atomic coordinates by using the chain rule.
(b) Do the same for Jacobi coordinates.

53. In Lagrangian mechanics one defines momenta $p_1, \ldots, p_n$ conjugate to $q_1, \ldots, q_n$ by $p_i = \partial T/\partial \dot{q}_i$. Show that the formulas in Problem 52 can be derived by writing T in terms of the new conjugate momenta and letting p_i be $i^{-1}\,\partial/\partial q_i$.

†54. Fill in the details of the proof of part (a) of Theorem XI.38.

†55. Prove that

$$\lim_{\min|a_i - a_j| \to \infty} \int_0^\infty \|(I_{D'} - I_{D''D'})e^{+iH_{D''D'}t}U_D(\mathfrak{a})e^{-iH_Dt}\psi\|\,dt = 0$$

if $\psi \in D(\tilde{H}_0)$, and thereby complete the proof of (77b).

†56. Use Theorem XI.39 to prove Theorem XI.40.

*57. Suppose that $V \in L^p \cap L^{3/2}(\mathbb{R}^3)$ with $1 < p < \frac{3}{2}$. By mimicking our proof of Theorem XI.41, prove an analogous theorem for $H = H_0 + V$.

58. Construct a function f, analytic in $\{z \,|\, \text{Im } z > 0\}$, continuous in $\{z \,|\, \text{Im } z \geq 0\}$ so that $z = 0$ is a limit point of zeros of f. (*Hint:* $\cos z$ has $z = \infty$ as a limit point of zeros.)

59. Using the Schwarz reflection principle, show that if f is analytic in $\{z \,|\, \text{Im } z > 0\}$, continuous in $\{z \,|\, \text{Im } z \geq 0\}$, then $\mathscr{E} = \mathbb{R} \cap \{z \,|\, f(z) = 0\}$ has an empty interior as a subset of $\mathbb{R}$.

†60. Let $V \in R$ and for $k \in \mathbb{R}$ let K_k be the operator on $L^2(\mathbb{R}^3)$ with kernel $K_k(x, y) = e^{ik|x-y|}(4\pi|x-y|)^{-1}|V(x)|^{1/2}V^{1/2}(y)$.
(a) Prove that $\text{Tr}(K_k^*K_k)$ is a constant.
(b) Using the Riemann-Lebesgue lemma, prove that $\text{Tr}(K_k^*K_k\,K_k^*K_k) \to 0$ as $k \to \infty$.
(c) Conclude that $\|K_k\| \to 0$ as $k \to \infty$.

Remark: This is a theorem of Klein and Zemach (see the notes to Section 6).

†61. (a) Let $V \in R \cap L^1(\mathbb{R}^3)$ and let $H_0 = -\Delta$; $H = H_0 + V$ (form sum). Prove that

$$(H-E)^{-1} = (H_0-E)^{-1} - [(H_0-E)^{-1}V^{1/2}][1 + |V|^{1/2}(H_0-E)^{-1}V^{1/2}]^{-1}[|V|^{1/2}(H_0-E)^{-1}]$$

for $E \notin \sigma(H)$. (*Hint:* See Problem 46.)
(b) Using the integral equation

$$G(x, y; E) = G_0(x, y; E) - \int G_0(x, z; E)V(z)G(z, y; E)\,dz$$

prove that $G(\cdot, y; E) \in L^1$ for almost all y. (*Hint:* Use (a) to prove that $V^{1/2}G \in L^2$ a.e. in y.)

†62. Let $V \in R$ and let $H = H_0 + V$ (form sum). Suppose that $H\psi = E\psi$ for $E = k^2 \geq 0$ and ψ in $L^2(\mathbb{R}^3)$. Let $\varphi = |V|^{1/2}\psi$. Prove that

$$\varphi(x) = -\int |V(x)|^{1/2}\frac{e^{ik|x-y|}}{4\pi|x-y|}V(y)^{1/2}\varphi(y)\,dy$$

Conclude that $E \in \mathscr{E}$, the exceptional set.

†63. Fill in the details in the proof of Lemma 5 used in the proof of Theorem XI.41.

*64. Suppose that $V(x) \leq 0$ for all x and $V \in L^1 \cap R$. Suppose that $-\Delta + V$ has a negative eigenvalue. Prove that the Born series for $T(0, 0)$ is not convergent.

65. The purpose of this problem is to prove (98).
(a) By using the scaling relation

$$G_0(x, y; E) = \lambda^{2-n}G_0(\lambda x, \lambda y; \lambda^2 E)$$

for $\lambda > 0$, show that it suffices to consider the case $|\text{Re } E| > 0$, $|E| = 1$.
(b) Write $G_0 = G_1 + G_2$ where

$$G_1 = (2\pi)^{-n}\int_{|p| \leq (1+\varepsilon)^2} (p^2 - E)^{-1}e^{ip\cdot(x-y)}\,d^np$$

for some $\varepsilon > 0$. Prove that G_2 is analytic in the region $|E| < 1 + \varepsilon$ for each fixed $x \neq y$ and that $|G_2(x, y; E)| \leq |x-y|^{-(n-2)}$; $n \geq 3$.
(c) By shifting the contour of integration for $|p|$ in G_1, complete the proof of (98).
(d) Prove the $n = 1, 2$ analogues of (98) as described in the text.
(e) Prove the $\partial_i(-\Delta - k^2)^{-1}$ results by finding and proving an analogue of (98).

66. Let $H = -\alpha\,\nabla\cdot\beta\,\nabla\alpha = -f\Delta + g\cdot\nabla + h = -f_0\Delta + V$ as in Theorem XI.45. Let $H_0 = -f_0\Delta$ and $W = g\cdot\nabla + h$.
(a) Prove that $\|W\varphi\| \leq \varepsilon\|H_0\varphi\| + c_\varepsilon\|\varphi\|$ for any $\varepsilon > 0$ and that $\|W\varphi\| \leq \varepsilon\|-f\Delta\varphi\| + c_\varepsilon\|\varphi\|$.
(b) Prove that $\|-f\Delta\varphi\| \leq (1+\varepsilon)\|H\varphi\| + c_\varepsilon'\|\varphi\|$.
(c) Prove that $\|(H - H_0)\varphi\| \leq a(\|H\varphi\| + \|H_0\varphi\|) + c\|\varphi\|$ for some $a < 1$.
(d) Conclude that H is self-adjoint on $D(H_0)$ by using Theorem X.13.

*67. Use the method described at the end of the appendix to Section 6 to prove an eigenfunction expansion for $-\Delta + V$ on $L^2(\mathbb{R}^3)$ if V falls off exponentially.

*68. (a) Let $\langle M, \mu\rangle$ be a measure space and suppose that $K(x, y)$ and $F(x)K(x, y)F(y)^{-1}$ are in $L^2(M \times M, d\mu \otimes d\mu)$ for some F which is finite and nonzero almost everywhere. Let ψ be an L^2 solution of $\psi(x) = \int K(x, y)\psi(y)\, dy$. Prove that $F\psi \in L^2(M, d\mu)$.

†(b) Let M_k be the kernel given by (102c) and let K_k be the kernel of $|V|^{1/2}(H_0 - k^2)^{-1}V^{1/2}$. Prove that $(1 - M_k)$ is invertible if and only if $(1 - K_k)$ is invertible.

†69. Let V be a Rollnik potential, let $E < 0$, and let $H = H_0 + V$ as a form sum. Prove that $(H_0 + V)\psi = E\psi$ for some nonzero $\psi \in D(H)$ if and only if

$$(|V|^{1/2}(H_0 - E)^{-1}V^{1/2})\varphi = -\varphi$$

for some nonzero $\varphi \in L^2$ and that ψ and φ are related by $\varphi = |V|^{1/2}\psi$.

Reference for Problems 68, 69: Simon's monograph (see the notes to Section 6), pp. 149–150, 81–83.

†70. (a) Suppose that $e^{\alpha|x|}V(x) \in R$ for some $\alpha > 0$. Prove that $e^{\beta|x|}V(x) \in L^1(\mathbb{R}^3)$ for any $\beta < \alpha$.

(b) Suppose that $V \in R + L^\infty$ has compact support. Prove that V is in R.

†71. Prove that the poles of $(1 - M_k)^{-1}$ where M_k is given by (102c) are simple poles.

†72. Fill in the details in the proof of the corollary to Theorem XI.46.

†73. Use Theorem XI.42 to verify equation (105).

74. Let H be an N-body Hamiltonian so that every cluster Hamiltonian has no nondiscrete eigenvalues. Let $E = \inf \sigma(H)$. Verify that $[E, \infty) = \bigcup_{n=1}^{\infty} I_n$ where the I_n are disjoint intervals so that $\mathscr{G}_E$, the family of open channels at energy E, is constant on each I_n.

†75. Verify the properties (1)–(3) and (1')–(3') of $F_V(E)$ used in the proof of Theorem XI.49.

†76. Prove that the map $\langle V, E\rangle \mapsto K_V(E)$ from $R \times \mathbb{R}_+ \to \mathscr{I}_2$ (with R the Rollnik class) is jointly continuous.

†77. Prove part (c) of Theorem XI.49, that is, that when V is Rollnik, the T operator $T(E)$ goes to zero in norm as $E \to \infty$. (*Hint:* Consult the discussion of convergence of the Born series at high energy in Section 6 and see Problem 60.)

†78. Use the dominated convergence theorem to verify (118) when $V \in C_0^\infty$.

†79. (a) Verify the uniqueness of solutions of the variable phase equation (120) away from $r = 0$ by using uniqueness results from Section V.6.

(b) Prove that local solutions of the variable phase equation (120) extend to all of $(0, \infty)$ by verifying that d cannot go to infinity at any finite point.

(c) Use the variable phase equation to prove that any solution obeying $\lim_{r\to 0} |r^{-1}d(r)| < \infty$ actually obeys $\lim_{r\to 0} r^{-1}d(r) = 0$.

(d) Prove the existence and uniqueness of solutions near $r = 0$ by setting up a suitable contraction map.

80. Indicate the k-dependence in the variable phase equation by writing $d(r, k)$.

(a) Prove that $d(r, k)$ is continuous in k for each fixed r. (*Hint:* Use the existence proof.)

(b) Prove that $d(r, k) \to d_\infty(k)$ as $r \to \infty$ locally uniformly in k so that $d_\infty(k)$ is continuous. (*Hint:* Use the variable phase equation and the bound $\int_1^\infty |V(x)|\, dx < \infty$.)

(c) Prove that $d_\infty(k) \to 0$ as $k \to \infty$. (*Hint:* Prove it first for sufficiently small r and then use the variable phase equation and $\int_1^\infty |V(x)|\, dx < \infty$.)

(d) Conclude that $d_\infty(k) = \delta_0(k)$ without any π ambiguity.

†81. Derive (123) from (122).

82. Prove Corollary 2 to Theorem XI.54. (*Hint:* Use the methods of Problem 80.)

†83. In the context of Theorem XI.55, prove that if $\lim_{r\to\infty} u'(r) \neq 0$, then

$$\lim_{k\to 0} \frac{\delta_0(k^2) - m\pi}{k} = \lim_{r\to\infty} \frac{u(r) - ru'(r)}{u'(r)}$$

†84. (a) Prove the uniqueness statement of Theorem XI.56.

(b) Under the stronger hypothesis that $\int_0^1 |V(x)|\, dx < \infty$, prove the stronger uniqueness statement that the regular equation has a unique solution which remains bounded as $x \to 0$.

†85. (a) Prove that $|\sin u| \leq [2|u|/(1 + |u|)]e^{|\operatorname{Im} u|}$ for all $u \in \mathbb{C}$.

(b) By writing

$$\frac{\sin k(x - y)}{k} = \frac{(\sin kx)e^{-iky} - e^{-ikx}\sin ky}{k}$$

prove that

$$\left|\frac{\sin k(x - y)}{k}\right| \leq \frac{4y}{1 + |k|y} \exp[|\operatorname{Im} k|y + (\operatorname{Im} k)x]$$

for $0 \leq x \leq y$.

(c) Using the estimates in (a) and (b) fill in the details in the proof of Theorem XI.57.

†86. Prove Levinson's theorem in case $\eta(0) = 0$ by using Jost function methods. (*Hint:* Prove the simplicity of the zero at $k = 0$.)

87. Let S be a Borel set in $\mathbb{R}$. Let $A(S)$ be multiplication by x on $L^2(S, dx)$. Prove that:

(a) $A(S)$ is unitarily equivalent to $A(T)$ if and only if $S\,\Delta\,T$ has Lebesgue measure zero.

(b) The spectrum of $A(S)$ is $\bar{S}$.

(c) If there exists an isometry U with $A(S)U = UA(T)$, then $T\backslash S$ has Lebesgue measure zero.

(d) Under the hypothesis of (c), suppose also that T is closed and $\sigma(A(S)) = \sigma(A(T))$. Then U is unitary.

(e) If A is any operator with simple and purely absolutely continuous spectrum, then A is unitarily equivalent to some $A(S)$. S is called the **essential support of** A.

88. Let H and H_0 be two operators with simple spectrum. Suppose that $\sigma_{ac}(H) \subset \sigma_{ac}(H_0)$, that the essential support (see Problem 87) of the absolutely continuous part of H_0 is closed and that $\Omega^\pm(H, H_0)$ exist. Prove that $\Omega^\pm(H, H_0)$ are complete. Does the result still hold if the hypothesis on the essential support is removed?

†89. (a) Prove that a locally uniform limit of harmonic functions is harmonic. (*Hint:* Prove convergence as distributions and use elliptic regularity, or use Poisson's formula.)

(b) Prove that local L^1 convergence of harmonic functions implies local uniform convergence. (*Hint:* Use the mean-value property.)

†90. (a) If $z = \cos\theta$ with $\theta = x + iy$, prove that $|y| = a$ is the ellipse with foci ± 1 and semimajor axis $\cosh a$ by using the formula $\cos\theta = (\cos x)(\cosh y) + i(\sin x)\times(\sinh y)$.

(b) If $z \in \mathbb{C}\backslash(-1, 1)$ and x is small, prove that $\sum_{\ell=0}^{\infty} x^\ell Q_\ell(z) = g(x, z)$ where

$$g(x, z) = \frac{1}{u}\ln\left[\frac{z - x + u}{(z^2 - 1)^{1/2}}\right] = \frac{1}{2u}\ln\left[\frac{1 - (x - u)^2}{1 - (x + u)^2}\right]$$

and $u = (1 - 2zx + x^2)^{1/2}$.

(c) Prove that $g(x, z)$ has radius of convergence in x given by $e^{+|\operatorname{Im}\theta|}$ where $\theta = \cos^{-1}(z)$.

(d) Let D be a compact set outside the canonical ellipse $|\operatorname{Im}\theta| = \ln H$. Show that $\sup_{\ell; z\in D} |Q_\ell(z)H^\ell| < \infty$.

91. Prove (c) of Theorem XI.63. (*Hint:* Prove that $\lim_{\ell\to\infty} |P_\ell(z)|^{1/\ell} = e^{-|\operatorname{Im}\theta|}$ where $\theta = \cos^{-1}(z)$.)

*92. (a) Let $A = -d^2/dx^2$ on $L^2(-\infty, \infty)$. Let B_1 (respectively, B_2) be $-d^2/dx^2$ on $L^2(0, \infty)$ (respectively, $L^2(-\infty, 0)$) with zero boundary conditions at zero, and let $B = B_1 \oplus B_2$. Find explicit formulas for $(A + 1)^{-1}$ and $(B + 1)^{-1}$ and conclude that $0 \le (B + 1)^{-1} \le (A + 1)^{-1}$ (operator inequality).

(b) Prove that $(B + 1)^{-1/2}(A + 1)^{1/2}$ is bounded and conclude that $\partial(B_1 + 1)^{-1/2}$ is bounded (where $\partial f = \partial f/\partial r$) and that $W(B_1 + 1)^{-1/2}$ is trace class if $W \in L^2_\delta(\mathbb{R})$ for $\delta > \frac{1}{2}$ (See Theorem XI.21.)

(c) Let $V = \partial W - W\partial =$ multiplication by $\partial W/\partial r$. Under the hypothesis that $W \in L^2_\delta(\mathbb{R})$, prove that V is a form-bounded perturbation of B_1 with relative bound zero and that $(B_1 + V + i)^{-1} - (B_1 + i)^{-1}$ is trace class.

(d) Let W be a function of $|x|$ on $\mathbb{R}^n$ with $\int |W(r)|^2(1 + r^2)^{-\frac{1}{2}-\varepsilon}\, dr < \infty$ for some $\varepsilon > 0$. Let $V = \partial W/\partial r$. Prove that $\Omega^\pm(-\Delta + V, -\Delta)$ exist and are complete.

†93. (a) Prove the bound $|u_n'(x)| \le n\gamma^n\|u_0\|A(x)$ needed in the proof of the proposition in Appendix 2 to Section 8.

(b) Extend the proof of the proposition to the case where $u_0(x)$ is x-dependent.

94. Let u obey (151). Prove that for all $f \in L^2(0, \infty)$ which have compact support in $(0, \infty)\backslash\mathscr{E}$, $\int f(k)u(k, r)\, dk \in L^2(0, \infty)$. (*Hint:* Write the integral in the two pieces suggested by (151). Control the $(1 + |r|)^{-\frac{1}{2}-\gamma}$ term by using $f \in L^1$ and the other term by the Plancherel theorem.)

*95. (a) Suppose that u obeys (151) and in addition that

$$\left|\frac{\partial u}{\partial r}(r, k) - k\cos\left(kr - \frac{\ell\pi}{2} + \delta_\ell(k)\right)\right| \le c(k)(1 + |r|)^{-\frac{1}{2}-\gamma} \tag{356}$$

Prove that if f is as in Problem 94, then $Y_{\ell m}(\hat{x})\int (kx)^{-1}f(k)u(kx)\, dk$ is in the form domain of $-\Delta$.

(b) If (356) holds, show that "$-\Delta + V$ essentially self-adjoint on C_0^∞" can be replaced by "C_0^∞ is a form core for $H = -\Delta + V$ and $Q(H) = Q(-\Delta)$" in the hypotheses of Theorem XI.69.

(c) Apply the extension given in (b) to the potential $(1 + |r|^2)^{-1}e^r\cos(e^r)$.

†96. Provide the details of the proof of Theorem XI.70.

97. (a) Let $A(y)$ and $T(y)$ be matrix-valued functions so that $T(y)$ is invertible, $\|T(x)T(y)^{-1}\| \le 1$, if $x \le y$, and so that $\tilde{A}(y) = T(y)A(y)T(y)^{-1}$ obeys $\int_{\mathbb{R}}^{\infty} \|\tilde{A}(y)\|\, dy < 1$. Suppose that $T(y)u_0 = u_0$ for all y. Show that $u(x) = u_0 + \int_x^\infty A(y)u(y)\, dy$ has a solution. (*Hint:* Estimate $T(x)u_n(x)$ inductively.)

(b) Let $f(x)$ be a positive monotone increasing function and $\tilde{A}$ a 2×2 matrix in L^1. Show that

$$\dot{u}(t) = -\begin{pmatrix} \tilde{a}_{11}(t) & \tilde{a}_{12}(t)f(t) \\ \tilde{a}_{21}(t)f(t)^{-1} & \tilde{a}_{22}(t)\end{pmatrix}u(t)$$

has a solution approaching $\langle 1, 0\rangle$ at infinity.

(c) Construct a solution of

$$-u''(x) + x^{2n}u(x) = 0$$

which is asymptotic to $\exp(-(n + 1)^{-1}x^{n+1})$ as $x \to \infty$. (*Hint:* Use variation of parameters with the two solutions $\exp(\pm(n + 1)^{-1}x^{n+1})$.)

(d) Suppose that $A = A_1 + A_2$ where $\tilde{A}_1(y) = T(y)A_1(y)T(y)^{-1}$ is in L^1 and that $A_2(y) = dB(y)/dy$ with $\tilde{B}(y) = T(y)B(y)T(y)^{-1}$ obeying $\tilde{A}\tilde{B} \in L^1$ and $\tilde{B} \to 0$ at infinity. Suppose that $T(y)u_0 = u_0$. Show that $\dot{u}(t) = A(t)u(t)$ has a solution satisfying $u(t) \to u_0$ at infinity.

(e) Let $f(x)$ be a positive monotone increasing function so that $|\dot{f}(t)| \le ct^{-\alpha}|f(t)|$. $t \ge R$, $\alpha > 0$. Let $\tilde{A}(t)$ be a 2×2 matrix-valued function with $\tilde{A} = M_1 + \dot{M}_2$ where $M_1 \in L^1$, $\tilde{A}M_2 \in L^1$, $t^{-\alpha}M_2 \in L^1$, and $M_2 \to 0$ at infinity. Show that

$$\dot{u}(t) = \begin{pmatrix} \tilde{a}_{11}(t) & \tilde{a}_{12}(t)f(t) \\ \tilde{a}_{21}(t)f(t)^{-1} & \tilde{a}_{22}(t)\end{pmatrix}u(t)$$

has a solution converging to $\langle 1, 0\rangle$ at infinity.

98. (a) Let f and g be functions in $C^1(\mathbb{R})$ so that $fg' - gf'$ is everywhere nonvanishing. Suppose that $\langle u(x), u'(x)\rangle$ and $\langle a(x), b(x)\rangle$ are related by the formulas:

$$u(x) = a(x)f(x) + b(x)g(x)$$

$$u'(x) = a(x)f'(x) + b(x)g'(x)$$

Let $W(x)$ be given. Prove that the differential equation $u''(x) = W(x)u(x)$ is equivalent to the differential equation $\rho'(x) = \Delta(x)\rho(x)$ where $\rho(x) = \langle a(x), b(x)\rangle$ and

$$\Delta = (f'g - gf')^{-1}\begin{pmatrix} -g(-f'' + Wf) & -g(-g'' + Wg) \\ f(-f'' + Wf) & f(-g'' + Wg)\end{pmatrix}$$

(b) Prove Theorem XI.67c by using Problem 97e and part (a) with the choice

$$f(x) = x^{-\gamma_j/2\alpha_j}\cos(\alpha_j x/2)$$

$$g(x) = x^{\gamma_j/2\alpha_j}\sin(\alpha_j x/2)$$

99. Prove (155) and conclude that the ordinary wave operators do not exist in the Coulomb case. (*Hint:* First prove that $(1 - P_{ac}(H))e^{itH}e^{-itH_0} \to 0$ weakly. Then, using the fact that $U_D(t)^*e^{-itH}P_{ac}(H)$ converges, prove that $P_{ac}(H)e^{itH}e^{-itH_0} \to 0$ weakly.)

†100. Let $W(k, t)$, $P(k)$ be real-valued functions so that for each s and almost every k,

$$W(k, t+s) - W(k, t) \to sP(k)$$

as $t \to \pm\infty$. Prove that

$$\text{s-lim}_{t\to\pm\infty} \exp(iW(i\nabla, t)) \exp(-iW(i\nabla, t+s)) = \exp(-isP(i\nabla))$$

(*Hint:* Use dominated convergence.)

†101. Use the method of stationary phase to prove (159a).

102. Let $H_0 = -\Delta$; $H = -\Delta - \lambda r^{-1} + V_s$; $H' = -\Delta - \lambda r^{-1}$. Let $\varphi \in C_0^\infty$ with $\varphi \equiv 1$ near $r = 0$. Let $\tilde{H} = H_0 - \lambda(1-\varphi)r^{-1}$; $W = -\lambda r^{-1}\varphi$.
(a) Prove that $\Omega_D^\pm(H, H_0) = \Omega^\pm(H, H')\Omega_D^\pm(H', H_0)$ and conclude that to prove completeness of $\Omega_D^\pm(H, H_0)$ it suffices to prove completeness of $\Omega_D^\pm(H', H_0)$ and $\Omega^\pm(H, H')$.
(b) Suppose that $V_s(H_0+1)^{-m-1}$ is trace class. Prove that $V_s(\tilde{H}+E)^{-m-1}$ is trace class by proving that $D(H_0^{m+1}) = D(\tilde{H}^{m+1})$.
(c) Prove that $W(H_0+1)^{-m-1}$ is trace class for m large enough.
(d) Prove that $(\tilde{H}+E)^{-m} - (H'+E)^{-m}$ and $(\tilde{H}+E)^{-m} - (H+E)^{-m}$ are trace class if $V_s(\tilde{H}+E)^{-m-1}$ is trace class so long as m is sufficiently large.
(e) Prove that if $V_s(H_0+1)^{-m-1}$ is trace class, then $\Omega^\pm(H, H')$ exist and are complete.

Remark: $\Omega_D^\pm(H', H_0)$ are complete by an explicit eigenfunction expansion; see Dollard's basic paper quoted in the notes to Section 9.

103. Verify that in the long-range classical case $(\Sigma_+\backslash\Sigma_-) \cup (\Sigma_-\backslash\Sigma_+)$ has measure zero and that (167) holds for every $\langle x_0, p_0\rangle$ in $\Sigma_\pm$.

104. Use a contraction mapping argument of the type used in Section 2 to prove the existence of solutions of (172).

105. Prove that for almost all p_{in}, b_{in}, the corresponding long range solution $x(t)$ associated with (172) obeys $\lim_{t\to\infty} |x(t)| = \infty$. (*Hint:* Let G be the map of $\langle p_{in}, a\rangle$ into the solution associated with (172) at time $t = 0$. Prove that G is measure preserving.)

106. Fix $\alpha > 0$. Suppose that $\sup_x [(1+x)^{\alpha+|\beta|} |D^\beta(V_n - V)|] \to 0$ for $|\beta| \le 2$. Let $N = [1/\alpha]$.
(a) Prove that the function $z_N(p, t; V_n)$ converges uniformly in t for p in compact subsets of $\mathbb{R}^n\backslash\{0\}$ to $z_N(p, t; V)$.
(b) Prove that the solutions of (172) associated with V_n converge as $n \to \infty$ to that for V.
(c) Prove that the map $\tilde{S}$ of Theorem XI.73 converges as $n \to \infty$.
(d) Prove that if V_n is short-range, the $\tilde{S}$ defined with z_N is identical to part of the usual short-range S.

*107. Using Hörmander's results on solutions of the Hamilton–Jacobi equation, improve Herbst's analysis of classical long-range scattering via canonical transformations. *References:* The Hörmander paper and the second Herbst paper quoted in the notes to Section 9.

108. (a) Let $W(k, t)$ be a real-valued function so that for some fixed H, $e^{iHt}\exp(-iW(-i\nabla, t)) \to \Omega_D^+$ as $t \to -\infty$. Let P_D be the projection on Ran Ω_D^+. Prove that for any other measurable function $\tilde{W}(k, t)$, there is an L^∞ function $G(k)$ and a subnet $t_\alpha \to -\infty$, so that

$$\text{w-lim}_{t_\alpha\to-\infty} P_D e^{iHt} \exp(-i\tilde{W}(-i\nabla, t_\alpha)) = \Omega_D^+ G(-i\nabla)$$

(*Hint:* Let $G(k)$ be a limit point of $\exp(iW(k, t) - i\tilde{W}(k, t))$ in the $\sigma(L^\infty, L^1) = w^*$-topology.)
(b) If $\text{s-lim}_{t\to-\infty} e^{iHt}\exp(-i\tilde{W}(-i\nabla, t)) = \tilde{\Omega}_D^+$ exists, prove that $P_D\tilde{\Omega}_D^+ = \Omega_D^+ G(-i\nabla)$.
(c) If, moreover, $P_D = P_{ac}(H)$, prove that $|G(k)| = 1$ a.e.

109. Let V obey $|D^\alpha V(x)| \le C(1+x)^{-|\alpha|-\varepsilon}$ for all α with $|\alpha| \le 3$. Prove that one can write $V = V_1 + V_2$ where $|V_2(x)| \le C(1+x)^{-1-\varepsilon}$ and $|(D^\alpha V_1)(x)| \le C(1+x)^{-m(|\alpha|)}$ where $m(\ell) = +\ell + \varepsilon$ for $\ell = 0, 1, 2, 3$ and $m(\ell) = 3 + \varepsilon + \frac{2}{3}(\ell - 3)$ for $\ell \ge 3$, by the following steps:
(a) Pick $\psi \in C_0^\infty(\mathbb{R}^n)$ with $\psi(x) = 1$ if $|x| \le 1$, $\psi(x) = 0$ if $|x| \ge 2$, and $0 \le \psi(x) \le 1$ for all x. Let $\psi_\nu(x) = \psi(2^{-\nu}x) - \psi(2^{1-\nu}x)$ and $V_\nu = V\psi_\nu$. Prove that $\|D^\alpha\psi_\nu\|_\infty \le C_\alpha 2^{-\nu|\alpha|}$, that $|(D^\alpha\psi_\nu)(x)| \le d(1+|x|)^{-|\alpha|}$ and conclude that $|D^\alpha V_\nu(x)| \le C(1+x)^{-|\alpha|-\varepsilon}$, $0 \le \alpha \le 3$.
(b) Let $\delta = \frac{2}{3}$. Let $\chi \in C_0^\infty(\mathbb{R}^n)$ with $\int \chi(x)\,dx = 1$ and $\int |x|^\beta\chi(x)\,dx = 0$ for $0 < |\alpha| < 3$. Let $\chi_\nu(y) = 2^{-\delta n\nu}\chi(2^{-\nu\delta}y)$. Prove that

$$\left| V_\nu(x-y) - V_\nu(x) - \sum_{1\le|\alpha|\le 2} (\alpha!)^{-1}(y)^\alpha (D^\alpha V_\nu)(x) \right| \le C|y|^3(1+x)^{-3-\varepsilon}$$

for all x, y with $x \in \text{supp } V_\nu$ and $y \in \text{supp } \chi_\nu$. Conclude that

$$|\chi_\nu * V_\nu(x) - V_\nu(x)| \le C(1+x)^{-1-\varepsilon}$$

(c) Prove that $D^\alpha(V_\nu * \chi_\nu) \le C_\alpha(1+x)^{-m(|\alpha|)}$.
(d) Complete the proof by taking $V_1 = \sum_\nu V_\nu * \chi_\nu$ and $V_2 = V - V_1$.

110. By following the method of Problem 109, show that if $|D^\alpha V(x)| \le C(1+x)^{-|\alpha|-\varepsilon}$, $|\alpha| \le M$ where $\varepsilon > \frac{1}{2}$ for $M = 1$ and $\varepsilon > \frac{1}{5}$ for $M = 2$, then $V = V_1 + V_2$ where $|V_2(x)| \le C(1+x)^{-1-\varepsilon}$ and $|(D^\alpha V_1)(x)| \le C(1+x)^{-m(|\alpha|)}$ where $m(1) + m(3) > 4$.

Reference for Problems 109 and 110: Hörmander's paper quoted in the notes to Section 9.

111. (a) Compute the classical Coulomb differential cross section (Rutherford cross section).
(b) Compute the Coulomb cross section in the Born approximation.

†112. Using the notation of Theorem XI.75 in Section 10, show that
(a) $\langle u, v\rangle \in P_{ac}(A_0) \Leftrightarrow B_0 u \in P_{ac}(B_0)$ and $v \in P_{ac}(B_0)$.
(b) $T_0 P_{ac}(A_0) = \begin{pmatrix} P_{ac}(B_0) & 0 \\ 0 & P_{ac}(B_0) \end{pmatrix}$.

†113. Assuming that Theorems XI.75 and XI.76 continue to hold if H_0 and H_1 have point spectrum at zero, fill in the details of the proof of the existence of the wave operators for optical scattering in inhomogeneous media (Example 2 of Section 10).

114. Using the methods of Section 10, develop a scattering theory for the wave equations

$$u_{tt} - \Delta u = 0$$

$$u_{tt} - \Delta u + q(x)u = 0$$

under appropriate conditions on $q(x)$.

115. Let A and B be bounded operators on a Hilbert space $\mathscr{H}$.
(a) Prove that $\sigma(AB)\backslash\{0\} = \sigma(BA)\backslash\{0\}$.
(b) Prove the commutation formula (205).

**116.* The purpose of this problem is to extend Theorems XI.79 and XI.80 to $n \neq 3$ dimensions.
(a) Use the method of proof of Theorem XI.21 to prove that $(1 + x^2)^{-\alpha}(1 + p^2)^{-\beta} \times (1 + x^2)^{-\gamma} \in \mathscr{I}_p$ as operators on $L^2(\mathbb{R}^n)$ so long as $\beta > n/2p$, $\alpha + \gamma > n/2p$ where α or γ may be negative. (*Hint:* Consider first the case $p \geq 2$ and then write

$$(1 + x^2)^{-\alpha}(1 + p^2)^{-\beta}(1 + x^2)^{-\gamma}$$

$$= [(1 + x^2)^{-\alpha}(1 + p^2)^{-\beta/2}(1 + x^2)^{-\delta}][(1 + x^2)^{\delta}(1 + p^2)^{-\beta/2}(1 + x^2)^{-\gamma}]$$

for suitable δ.)
(b) Let $R_0 = (H_0 + 1)^{-1}$ and let R be another operator. Suppose that $(1 + x^2)^k \times (R - R_0)(1 + x^2)^k \in \mathscr{I}_p$ for $p > \frac{1}{2}n$ and all k. Prove inductively that $(1 + x^2)^k \times (R^m - R_0^m)(1 + x^2)^k \in \mathscr{I}_p$ for all k, all $m = 1, 2, 3, \ldots$ and $p > n/2m$ and in particular that $R^m - R_0^m \in \mathscr{I}_1$ if $m > n/2$.
(c) Prove suitable analogs of Theorems XI.79 and XI.80 for any n.

117. We say that positive self-adjoint operators A and B obey $A \leq B$ if and only if $Q(B) \subset Q(A)$ and $(\varphi, A\varphi) \leq (\varphi, B\varphi)$ for all $\varphi \in Q(B)$. Suppose that A and B have bounded inverses. Prove that $B^{-1} \leq A^{-1}$. *Hint:*

$$(\varphi, B^{-1}\varphi) \leq (A^{-1}\varphi, AB^{-1}\varphi)$$

$$\leq (A^{-1}\varphi, \varphi)^{1/2}(B^{-1}\varphi, AB^{-1}\varphi)^{1/2}$$

$$\leq (\varphi, A^{-1}\varphi)^{1/2}(\varphi, B^{-1}\varphi)^{1/2}.$$

†*118.* Fill in the details of the proof of Theorem XI.81′.

119. Let W be a bounded closed subset of $\mathbb{R}^2$ and let $\Gamma = \{\langle x_1, x_2, x_3\rangle \in \mathbb{R}^3 \mid \langle x_1, x_2\rangle \in W, x_3 = 0\}$. The purpose of this problem is to prove that $R^2_{\Gamma;N} - R_0^2$ is trace class.
(a) Show that Theorem XI.80 can be modified to allow the sphere S to be replaced by the boundary of a cube C.
(b) Let C be a cube and let Γ' be a piece of hyperplane slicing C into two rectangular parallelopipeds. Prove, that $\tilde{R}_{\partial C \cup \Gamma;N}$, the Laplace operator on $L^2(C)$ with Neumann boundary conditions on $\partial C \cup \Gamma'$, is Hilbert-Schmidt. (*Hint:* Compute the eigenvalues of $\tilde{R}$!)
*(c) Complete the proof that $R^2_{\Gamma;N} - R_0^2$ is trace class.

120. In the case of Dirichlet obstacle scattering, we showed that $\Omega^{\pm}(A_D, A_0; I^*_{10})$ exist. Let J be multiplication (on both components) by a function $\varphi \in C_0^\infty$ vanishing in a neighborhood of the obstacle. Show that $\Omega^{\pm}(A_D, A_0; J)$ exist.

121. Prove uniqueness of the representations in Theorem XI.82 and XI.83.

122. (a) Let $dv(\theta)$ be a translation invariant Borel measure on the circle. Prove that $dv = c\, d\theta$. (*Hint:* Apply Fubini's theorem to $\int f(\theta + \theta')\, dv(\theta)\, d\theta'$.)
(b) Let $dv(x)$ be a translation invariant Borel measure on $\mathbb{R}$. Prove that $dv(x) = c\, dx$.

†*123.* Prove that the operator valued function $t(\sigma + iy)$ is norm analytic in the upper half-plane by using the fact that it is weakly analytic and the ideas of Theorem VI.4.

**124.* Using the ideas in Example 3 of Section 11, verify the hypotheses of Theorem XI.91 for the interacting group of Example 2.

125. Under the additional hypothesis $q > 1$ in Theorem XI.98, prove that $\|e^{iAt}\varphi(t) - \varphi_+\|_{\text{scat}} \to 0$ as $t \to +\infty$.

†*126.* Prove that the scattering operator on small data constructed in Theorem XI.98 is one to one. (*Hint:* Turn around the uniqueness part of Theorem XI.97.)

127. (a) Let g be a positive integrable function on $\mathbb{R}$ and suppose that f is measurable, bounded on each interval $(-\infty, t)$, and satisfies

$$f(t) \leq c_0 + b_0 \int_{-\infty}^{t} f(s)g(s)\, ds \qquad \text{for all } t$$

Prove that

$$f(t) \leq c_0 \exp\left(b_0 \int_{-\infty}^{t} g(s)\, ds\right) \qquad \text{for all } t$$

*(b) Let α and β be two Hermitian two by two matrices that satisfy

$$\alpha^2 = I = \beta^2, \qquad \beta\alpha + \alpha\beta = 0$$

Prove global existence for the coupled Klein-Gordon and Dirac equations in one dimension:

$$\frac{\partial \psi}{\partial t} + i\left(i\alpha \frac{\partial}{\partial x} - m_e\beta\right)\psi = -ig\beta u\psi$$

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + m_0^2 u = \bar{\psi} \cdot \beta\psi$$

where g is a real coupling constant, $u(x, t)$ is a real-valued function on $\mathbb{R}^2$, $\psi(x, t)$ is a $\mathbb{C} \times \mathbb{C}$ valued function on $\mathbb{R}^2$, and $\bar{\psi} \cdot \beta\psi$ denotes the dot product. (*Hint:* Find conserved quantities, use the Sobolev estimate $\|f\|_\infty \leq c\|f'\|_2^{1/2}\|f\|_2^{1/2}$, and iterate like mad.)

Reference: J. Chadam, "Global solutions of the Cauchy problem for the (classical) coupled Maxwell-Dirac equations in one space dimension," *J. Functional Anal.* **13** (1973), 173–184.

†*128.* Fill in the details of the proof of Theorem XI.100. In particular:
(a) Show that for each t and η, M_t is uniformly continuous on $\{\psi \in \Sigma_{\text{scat}} \mid \|\psi\|_{\text{scat}} \leq \eta\}$ in the $\|\cdot\|_{\text{scat}}$ topology. (*Hint:* First show that M_t is continuous in the $\|\cdot\|$ topology.)
(b) Prove that Ω^+ is one-to-one.

129. (a) Let $B = \sqrt{-\Delta + m^2}$ on $L^2(\mathbb{R}^3)$. Show that there is a constant c so that

$$\|B^{-1} \sin[(t-s)B]u^3(s)\|_\infty \leq C\|Bu(s)\|_2 \|u(s)\|_\infty^2$$

for each $u(s) \in D(B^2) \subset L^2(\mathbb{R}^3)$.

(b) Use this estimate and the techniques of Theorem XI.100 to construct the wave operators for

$$u_{tt} - \Delta u + m^2 u = -u^3$$

in the case $n = 3$.

130. Prove global existence for the nonlinear Schrödinger equation (261) for $p \geq 1$ and $\lambda > 0$.

Note: Problems 131, 132, 133 require some familiarity with the quantum theory of addition of angular momentum.

131. Let $\sigma^{(\alpha)}$ and $\sigma^{(\beta)}$ be Pauli spins at different sites in a Heisenberg model. Let $k_{\alpha\beta}$ be defined by $k_{\alpha\beta} = (\sigma^{(\alpha)} + \sigma^{(\beta)})^2$. Prove that $k_{\alpha\beta}$ has the eigenvalues 0 and 8 and that $\sigma^{(\alpha)} \cdot \sigma^{(\beta)} = 1$ when $k_{\alpha\beta} = 8$ and $\sigma^{(\alpha)} \cdot \sigma^{(\beta)} = -3$ when $k_{\alpha\beta} = 0$.

**132.* (a) Let $\sigma^{(\alpha)}$, $\sigma^{(\beta)}$, $\sigma^{(\gamma)}$ be three Pauli spins at different sites. Prove that

$$(1 - \sigma^{(\alpha)} \cdot \sigma^{(\beta)}) \leq 2(1 - \sigma^{(\alpha)} \cdot \sigma^{(\gamma)}) + 2(1 - \sigma^{(\beta)} \cdot \sigma^{(\gamma)})$$

as an operator inequality.

(b) Let $H = -\sum J_{\alpha\beta} \sigma^{(\alpha)} \cdot \sigma^{(\beta)}$ be a finite sum with each $J_{\alpha\beta} \geq 0$ so that the sites cannot be broken into two noninteracting groups. Prove that the lowest eigenvalue of H is $-\sum J_{\alpha\beta}$ and that this eigenvalue has multiplicity $n + 1$ where n is the number of sites. (*Hint:* Use (a) to prove that every eigenvector with eigenvalue $-\sum J_{\alpha\beta}$ has total angular momentum $S = \frac{1}{2}(\sum \sigma_\alpha)$ with $s = \frac{1}{2}n$.)

**133.* (a) Let $\sigma^{(\alpha)}$, $\sigma^{(\beta)}$ be Pauli spins at two different sites. Let ρ be a density matrix with $\mathrm{Tr}(\rho\sigma^{(\alpha)} \cdot \sigma^{(\beta)}) = 1$. Prove that $\mathrm{Tr}(\rho\sigma^{(\alpha)}) = \mathrm{Tr}(\rho\sigma^{(\beta)})$.

(b) Let $\psi \in \mathscr{H}_n$, the n spin space for the infinite volume system. Prove that

$$\lim_{\Lambda \to \infty} \left(\psi, \sum_{x \in \Lambda} \tfrac{1}{2}(\sigma_z^{(x)} + 1)\psi\right) = n$$

(c) Let H be the infinite volume Hamiltonian for the zero temperature Heisenberg model. Let $\psi \in \mathscr{H}_n$ with $H\psi = 0$. Prove that $(\psi, \sigma_z^{(\alpha)}\psi)$ is independent of α and conclude that $n = 0$.

†*134.* Verify (276).

**135.* Let $H_2(K)$ be the fibering described at the end of Section 14. Let $J_2(K)$ and $H_2^{(0)}(K)$ be the corresponding fibering for J_2 and $H_1^{\otimes}$. Prove that

$$H_2(K)J_2(K) - J_2(K)H_2^{(0)}(K)$$

is finite rank and thus trace class. Conclude that $\mathrm{Ran}\,\Omega_2^+ = \mathrm{Ran}\,\Omega_2^-$.

136. Show that the inner product (344) is well defined by showing that if v and w have different representations as finite linear combinations of vectors in D_0, then (v, w) is independent of the representation chosen.

†*137.* In the proof of Theorem XI.104, verify that the operators $h(t) + M + 1$ satisfy the hypotheses of Theorem X.70.

†*138.* Verify part (e) of Theorem XI.104.

†*139.* Check that the charged scalar field of mass m obeys the obvious extension of the Gårding-Wightman axioms.

†*140.* Generalize the causality proof in Section 15 to show that $[\varphi(f, t), \varphi(g, t')^*] = 0$ whenever $\{\langle x, t\rangle \mid x \in \mathrm{supp}\, f\}$ and $\{\langle x, t'\rangle \mid x \in \mathrm{supp}\, g\}$ are spacelike separated.

†*141.* Fill in the following details of the proof of Theorem XI.106:

(a) Complete the proof of (295).

(b) Prove that

$$(a_i + \lambda_i b_i^*)e^{-\lambda_i a_i^* b_i^*}\psi_{\mathrm{in}} = 0$$

(c) Fill in the details of the proof that S^{-1} is an isometry.

142. Fix a short-range potential V in $\mathbb{R}^3$. Let $\mathscr{F}$ be the Boson Fock space built on $L^2(\mathbb{R}^3)$, that is, $\mathscr{F}_n = L_s^2(\mathbb{R}^{3n})$, the functions $f(x_1, \ldots, x_n)$ on $\mathbb{R}^{3n}$ which are symmetric. Define a Hamiltonian H on $\mathscr{F}$ by requiring that H leave $\mathscr{F}_n$ invariant, V be even, and that

$$H \upharpoonright \mathscr{F}_n = -\sum_{i=1}^n \Delta_i + \sum_{i<j} V(x_i - x_j)$$

Let Ω_0 be the Fock vacuum and define a "field operator" by

$$\varphi(x, 0) = (2\pi)^{-3/2} \int [e^{-ip\cdot x}a^\dagger(p) + e^{+ip\cdot x}a(p)]\, d^3p/\sqrt{2}$$

$$\varphi(x, t) = e^{itH}\varphi(x, 0)e^{-itH}$$

By a regular wave packet for the free Schrödinger equation, we mean a function $f(x, t)$ of the form

$$f(x, t) = (2\pi)^{-3/2} \int e^{-ip^2t}e^{ip\cdot x}g(p)\, d^3p$$

with $g \in C_0^\infty(\mathbb{R}^3)$. Given such an f, define $\varphi_f(t)$ by

$$\varphi_f(t) = \int \varphi(x, t)f(x, t)\, d^3x$$

(a) Prove that for any regular wave packets $f_1, \ldots, f_n$,

$$\eta(t) \equiv \varphi_{f_1}(t) \cdots \varphi_{f_n}(t)\Omega_0$$

has a limit as $t \to \pm\infty$ in the norm topology by writing $\eta(t)$ as $e^{itH}e^{-itH_0}g$ for suitable g and using the known facts about nonrelativistic scattering.

(b) Prove (a) by mimicking the Haag-Ruelle method. (*Hint:* The TVEV at equal time are extremely simple; compute them exactly!)

(c) Suppose that $H \upharpoonright \mathscr{F}_2$ has a bound state. Introduce suitable new "field" operators ψ so that the procedure in (a) will yield channel wave operators with this bound state if ψ fields are used and channel wave operators for free particles and this bound state if φ and ψ are used.

References: The Hepp lectures and Sandhas article quoted in the notes to Section 16.

143. Prove that the TVEV are given explicitly in terms of the Wightman distributions by

$$\mathscr{W}_{n,T}(x_1, \dots, x_n) = \sum_{P \in \mathscr{P}_n} (-1)^{(|P|+1)} c_P \mathscr{W}_{k_1}(x_{i_1}, \dots, x_{i_k}) \cdots \mathscr{W}_{k_\ell}(x_{i_1'}, \dots, x_{i_{k'}'})$$

where $|P| = \ell$ and

$$c_P = \begin{cases} 1, & |P| = 1 \\ |P| - 1, & |P| \geq 2 \end{cases}$$

144. Suppose that for $n = 1, 2, \dots$ we are given functions $f_n(\lambda)$ on $(0, \infty)$ with asymptotic series $f_n(\lambda) \sim \sum_m a_{n,m} \lambda^m$. Define "truncated" functions $f_{n,T}(\lambda)$ inductively by

$$f_n(\lambda) = \sum N(m_1, \dots, m_k) f_{m_1,T}(\lambda) \cdots f_{m_k,T}(\lambda)$$

where $N(m_1, \dots, m_k)$ is the number of distinct partitions of $\{1, \dots, n\}$ into k sets with $m_1, \dots, m_k$ elements (so $N = n!/m_1! \cdots m_k!$ if the m_i are distinct but it is less if some m_i are equal). By an n, m graph, we mean a set of n labeled red points and m labeled black points joined together by some set of lines. To each graph Γ we define a value $V(\Gamma)$ with two restrictions: (i) The value is independent of permutation of the labels of the red (respectively, black) points. (ii) The value of any graph Γ which is a "union" of connected graphs $\Gamma_1, \dots, \Gamma_k$ is $V(\Gamma) = V(\Gamma_1) \cdots V(\Gamma_k)$. Suppose that

$$a_{n,m} = \sum_{\Gamma, \text{ an } n, m \text{ graph}} V(\Gamma).$$

Prove that $f_{n,T}(\lambda) \sim \sum a^T_{n,m} \lambda^m$ where

$$a^T_{n,m} = \sum_{\Gamma \text{ a connected } n, m \text{ graph}} V(\Gamma)$$

Remark: It is only for notational convenience that we did not let $f_n(\lambda)$ depend on n points $x_1, \dots, x_n$ obtaining a family of Wightman distributions and TVEVs in this way. The analogue of this result in that case has the following consequence: In those theories where the $\mathscr{W}_n$ are given "formally" as sums of Feynman diagrams, the TVEV are given as sums of connected Feynman diagrams. It also means that the "connected" S-matrix of Section 5 is related to the full S-matrix as the TVEV are related to the VEV.

†145. Verify (314). (*Hint:* Prove that $\mathbf{a} \cdot \mathbf{P}$ has purely absolutely continuous spectrum on $\{\psi_0\}^\perp$ and use the Riemann-Lebesgue lemma.)

†146. (a) Show that the support property of the $\hat{W}_n$ (Theorem IX.32) is equivalent to saying that the support of the $\hat{\mathscr{W}}_n$ is

$$S_n = \{\langle q_1, \dots, q_n \rangle | q_1 \in -\bar{V}_+, q_1 + q_2 \in -\bar{V}_+, \dots, q_1 + \cdots + q_{n-1} \in -\bar{V}_+, q_1 + \cdots + q_n = 0\}$$

(*Hint:* $\sum_{i=1}^n q_i x_i = \sum_{i=1}^{n-1} (x_i - x_{i+1})(\sum_{j=1}^i q_j) + x_n \sum_{j=1}^n q_j$.)

(b) Let $\langle i_1, \dots, i_{k_1} \rangle, \dots, \langle i'_1, \dots, i'_{k'} \rangle$ be a partition of $\{1, \dots, n\}$ with $i_1 < \cdots < i_{k_1}$; etc. Let

$$G(x_1, \dots, x_n) = \mathscr{W}_{k_1}(x_{i_1}, \dots, x_{i_{k(1)}}) \cdots \mathscr{W}_{k_\ell}(x_{i'_1}, \dots, x_{i'_{k(\ell)}})$$

Prove that $\hat{G}$ has support in S_n.

(c) If $\hat{\mathscr{W}}_{n,T}$ is used in (a), show that $-\bar{V}_+$ can be replaced by $-\bar{V}_{+,m}$ if Property 9 is assumed.

(d) Let $\langle q_1, \dots, q_n \rangle$ be in the support of $\hat{\mathscr{W}}_{n,T}(x_{i_1}, \dots, x_{i_k}, x_{i'_1}, \dots, x_{i'_{k'}})$. Prove that $\sum_{i \in I} q_i \in -\bar{V}_{+,m}$ and $\sum_{i \in I'} q_i \in \bar{V}_{+,m}$.

147. Prove Theorem XI.117 in the notes for scattering on C^*-algebras.

148. (a) With the notation of Theorem XI.114, show that

$$N^{-1} \sum_{n=0}^{N-1} |F(n)|^2 \to \sum_{x \in \mathbb{R}} |\mu(\{x\})|^2 \quad \text{as} \quad N \to \infty$$

(b) Let U be a unitary operator on a separable Hilbert space and let $\{E_i\}_{i=1}^M$ ($M = 1, \dots, \infty$) be its eigenvalues and P_i the corresponding eigenprojections. Show that for any vectors η, ψ,

$$\lim_{N \to \infty} N^{-1} \sum_{n=0}^{N-1} |(\eta, U^n \psi)|^2 = \sum |(\eta, P_i \psi)|^2$$

(c) Suppose that $U\varphi = \varphi$. Prove that

$$\lim_{N \to \infty} N^{-1} \sum_{n=0}^{N-1} |(\eta, U^n \psi) - (\eta, \varphi)(\varphi, \psi)| = 0$$

for all $\eta, \psi \in \mathscr{H}$ if and only if φ is the only eigenvector of U. (This is Theorem VII.14b.)

149. (a) Map $Q = \times_{n=1}^\infty \{-1, 1\}$ onto $[0, 1]$ by $Tx = \sum_{n=1}^\infty 3^{-n}(x_n + 1)$. Put the measure $\mu_0(\{1\}) = \mu_0(\{-1\}) = \frac{1}{2}$ on $\{-1, 1\}$ and the product measure μ on Q. Define ν on $[0, 1]$ by $\nu(A) = \mu(T^{-1}(A))$. Show that ν is the Cantor measure.

(b) Using (a), show that $F(t) = \int e^{ixt}\, d\nu(x)$ with ν the Cantor measure is given by

$$F(t) = e^{it/2} \prod_{n=1}^\infty \cos(3^{-n}t)$$

(c) Show that $F(3^N(2\pi))$ does not go to zero as $N \to \infty$ and conclude that $F(t) \not\to 0$ as $t \to \infty$.

(d) Let A be multiplication by x on $L^2(0, 1; d\nu)$. Show that $U(t) = e^{itA}$ does not go weakly to zero.

(e) If one maps Q onto $[0, 1]$ by $Sx = \sum_{n=1}^\infty 2^{-n-1}(x_n + 1)$, then $\nu(\cdot) = \mu(S^{-1}(\cdot))$ is just Lebesgue measure on $[0, 1]$. Why cannot one claim that $F(2^N(2\pi))$ does not go to zero?

(f) Prove that $t^{-1} \sin t = \prod_{n=1}^\infty \cos(2^{-n-1}t)$.

150. In the context of the Lax-Phillips theory suppose that one knows only that A_1 has purely continuous spectrum. Use Lemma 3 before Theorem XI.8 and the RAGE theorem to show that (219) holds.

151. Let V be $H_0(= -\frac{1}{2}\Delta)$-bounded and pick a fixed j with $1 - j \in C_0^\infty$, $j(x) = 1$ (respectively, 0) if $|x| \geq 1$ (respectively, $|x| \leq \frac{1}{2}$). Let $j_R(x) = j(x/R)$. For $z \notin \sigma(H_0)$, let

$$h(R, z) = \|V(H_0 - z)^{-1} F(|x| \geq R)\|,$$

$$h_1(R, z) = \|V(H_0 - z)^{-1} j_R\|, \qquad h_2(R, z) = \|V j_R (H_0 - z)^{-1}\|.$$

(a) Prove that $h(R, z) \leq h_1(R, z) \leq h(\frac{1}{2}R, z)$ and conclude that $h \in L^1(0, \infty; dR)$ if and only if $h_1 \in L^1$ for the same z.

(b) Use a commutator to prove that

$$|h_1(R) - h_2(R)| \leq C_z R^{-1} h_1(\tfrac{1}{2}R)$$

and prove that $h_1 \in L^1$ if and only if $h_2 \in L^1$ for the same z.

(c) Use the first resolvent formula to show that the condition $h_2 \in L^1$ is z-independent.
(d) Let V commute with each j_R. Prove that $h(R, z)$ is in L^1 if and only if $\|F(|x| \geq R)V(H_0 - z)^{-1}\|$ is in L^1.

152. (a) Extend the formulas (270n, o, p) for the current to accommodate several components $\{u_\alpha\}_{\alpha=1}^n$ with the possibility that V mixes components.
(b) An **internal symmetry** has the form $y = x$, $s = t$, V_α is a function of $\{u_\beta\}$ alone. Write a formula for the conserved quantity resulting from an internal symmetry.
(c) Let $\mathscr{L}(u) = |u_t|^2 - |\nabla u|^2 - G(u)$. Suppose that u is allowed to be complex-valued but that G is only a function of $|u|$. Find the conserved quantity Q (the conventional "charge") corresponding to the internal symmetry $u \to e^{it}u$.
(d) Let u be an n-component function and let $\mathscr{L}(u) = |u_t|^2 - |\nabla u|^2 - G(u)$. If $\mathscr{L}$ is a function only of $|u|$, write down the conserved quantities in case u is real-valued ($O(n)$-symmetry) or complex-valued ($U(n)$ symmetry). Suppose that $\mathscr{L}$ has a symmetry breaking term $-F(u_1)$ added to it. Compute the sources now introduced into the previously conserved currents.

153. (a) For the equation $u_{tt} = \Delta u - |u|^{p-1}u$, let k_0 be given by (270d) with $\frac{1}{4}u^4$ replaced by $(1/\rho + 1)|u|^{p+1}$. Find the source term in the corresponding broken conformal invariance.
(b) If $p > 3$, show that $S(u) \leq 0$ for $t > 0$.
*(c) For $3 < p < 5$, prove the analogue of Theorem XI.101.

154. Suppose that $\mathscr{L}(u)$ has the form $\partial_0 B_0 + \nabla \cdot \mathbf{B}$ for some local functions B_0, $\mathbf{B}$ of u. Show that every function obeys the corresponding Euler–Lagrange equations.

155. Find the other nine conserved quantities for (270b), i.e., the six Lorentz invariance charges and the other three conformal charges.

156. (a) Find the dilation current and source term for $u_{tt} = \Delta u - |u|^{p-1}u$ when $x \in \mathbb{R}^n$, $t \in \mathbb{R}$. Choose the transformation law on u such that $\delta\mathscr{L} = 0$ for the "free" case $u_{tt} = \Delta u$.
(b) Repeat this for the conformal charge.

Material Preprinted from Volume IV

The crucial (and often hardest) step in most proofs of asymptotic completeness for quantum systems is the proof that the interacting Hamiltonian has no singular continuous spectrum. Conversely, one of the best ways of showing that a self-adjoint operator has no singular continuous spectrum is to show that it is the interaction Hamiltonian of a quantum system with complete wave operators. This deep connection between scattering theory and spectral analysis shows how artificial the division of material into Volumes III and IV really is. Therefore, as an aid to readers whose primary interest is scattering theory, we have preprinted below three sections from Volume IV.

XIII.6 The absence of singular continuous spectrum I: General theory

Spectral analysis of an operator A concentrates on identifying the five sets $\sigma_{ess}(A)$, $\sigma_{disc}(A)$, $\sigma_{ac}(A)$, $\sigma_{sing}(A)$, $\sigma_{pp}(A)$. For large classes of Schrödinger operators H, we have succeeded in identifying $\sigma_{ess}(H)$ and $\sigma_{ac}(H)$. A precise determination of $\sigma_{disc}(H)$ is a detailed question, but we have seen how to use

the min-max principle to obtain a lot of information about it. That leaves $\sigma_{sing}(H)$ and $\sigma_{pp}(H)$. We shall discuss the question of proving $\sigma_{pp} = \sigma_{disc}$ in Section 13. The next five sections involve the difficult study of $\sigma_{sing}(H)$. Our discussion of asymptotic completeness in Section XI.3 suggests that $\sigma_{sing}(H) = \varnothing$ and our main goal will be the proof of this fact for various classes of Schrödinger operators.

As we have already emphasized, there are close connections between proving the absence of singular continuous spectrum and scattering theory. In fact, the development of eigenfunction expansions in Section XI.6 already tells us something about the singular spectrum. In general when $V \in L^1 \cap R$ we know that $\sigma_{sing} \subset \mathscr{E}$, the exceptional set, so that σ_{sing} has Lebesgue measure 0. And in two cases, first when $V \in L^1 \cap R$ and $\|V\|_R < 4\pi$, and secondly, if $Ve^{a|x|} \in R$ for some $a > 0$, we know that $\mathscr{E}$ is discrete so that $\sigma_{sing} = \varnothing$. In this section we shall develop a fundamental criterion for the absence of singular spectrum and show how it allows us to recover these two results from first principles without very much effort. In Sections 7 and 8, we shall use the connection between scattering theory and spectral analysis in reverse: The techniques developed to prove that there is no singular continuous spectrum will yield very strong results on asymptotic completeness.

The fundamental criterion for the absence of singular spectrum is very simple. In part it will depend on Stone's formula (Theorem VII.13):

$$\tfrac{1}{2}(\varphi, (E_{[a,b]} + E_{(a,b)})\varphi) = \lim_{\varepsilon \downarrow 0} \pi^{-1} \int_a^b \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx$$

where $R(\lambda)$ is the resolvent $(H - \lambda)^{-1}$ of some self-adjoint H and $\{E_\Omega\}$ is its family of spectral projections. In particular, one has that

$$\sup_{0<\varepsilon<1} \int_a^b |\operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)|^p\, dx < \infty \tag{30}$$

in the case $p = 1$ for any $\varphi \in \mathscr{H}$.

Theorem XIII.19 Let H be a self-adjoint operator with resolvent $R(\lambda) = (H - \lambda)^{-1}$. Let (a, b) be a bounded interval and $\varphi \in \mathscr{H}$. Suppose that there is a $p > 1$ for which (30) holds. Then $E_{(a,b)}\varphi \in \mathscr{H}_{ac}$.

Proof By Stone's formula and the fact that $E_{(c,d)} \leq E_{[c,d]}$

$$(\varphi, E_{(c,d)}\varphi) \leq \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \int_c^d \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx$$

for each open interval (c, d). Let S be an open set in (a, b) so that $S = \bigcup_{i=1}^{N} (a_i, b_i)$ is a union of disjoint open intervals. Suppose first that $N < \infty$. Then

$$\begin{aligned}(\varphi, E_S\varphi) &\leq \frac{1}{\pi} \sum_{i=1}^{N} \lim_{\varepsilon \downarrow 0} \int_{a_i}^{b_i} \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx \\ &\leq \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \sum_{i=1}^{N} \int_{a_i}^{b_i} \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx \\ &\leq \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \left[\int_a^b |\operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)|^p\, dx \right]^{1/p} |S|^{1/q} \\ &\leq C|S|^{1/q}\end{aligned}$$

where $|S|$ is the Lebesgue measure of S and q is the conjugate index to p. If N is infinite, let $S_m = \bigcup_{i=1}^{m} (a_i, b_i)$. Then

$$(\varphi, E_S\varphi) = \lim_{m \to \infty} (\varphi, E_{S_m}\varphi) \leq \lim_{m \to \infty} C|S_m|^{1/q} = C|S|^{1/q}$$

Let I be an arbitrary set of Lebesgue measure 0 inside (a, b). Since Lebesgue measure is outer-regular, we can find an open set $S^{(k)}$ with $I \subset S^{(k)}$ and $|S^{(k)}| < 1/k$. Thus

$$(\varphi, E_I\varphi) \leq \inf_k (\varphi, E_{S^{(k)}}\varphi) \leq C \inf_k |S^{(k)}|^{1/q} = 0$$

Thus the measure $\Omega \mapsto (\varphi, E_\Omega\varphi)$ is absolutely continuous on (a, b) so $E_{(a,b)}\varphi \in \mathscr{H}_{\text{ac}}$. ∎

Theorem XIII.20 Let H be a self-adjoint operator with resolvent $R(\lambda) = (H - \lambda)^{-1}$. Let (a, b) be a bounded interval. Suppose that there is a dense set D in $\mathscr{H}$ so that, for each $\varphi \in D$, (30) holds for some $p > 1$. Then H has purely absolutely continuous spectrum on (a, b), i.e., Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$. Conversely, if Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$, then there is a set D, dense in Ran $E_{(a,b)}$, so that (30) holds for any $p \geq 1$ including $p = \infty$ when $\varphi \in D$.

Proof The first half of the theorem follows from Theorem XIII.19. For the second half, let D be the set of vectors φ for which the spectral measure $d\mu_\varphi$ for H is of the form $f(x)\, dx$ where $f \in L^\infty$ with compact support in (a, b). By hypothesis, D is dense in Ran $E_{(a,b)}$. Moreover,

$$\operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi) = \int_{-\infty}^{\infty} g_\varepsilon(x - y) f(y)\, dy$$

where $g_\varepsilon(y) = \varepsilon(y^2 + \varepsilon^2)^{-1}$. Since $\|g_\varepsilon\|_1 = \pi$ independently of ε, (30) holds with $p = \infty$ by Young's inequality and thus for all p since (a, b) is finite. ∎

In most applications of Theorem XIII.20, one actually proves that $(\varphi, R(\lambda)\varphi)$ is bounded on $M = \{x + i\varepsilon \,|\, \varepsilon \in (0, 1),\ x \in (a, b)\}$ or more strongly that $(\varphi, R(\lambda)\varphi)$ has a continuous extension to $\bar{M}$. A typical application is:

Theorem XIII.21 Let $V \in R$, the Rollnik class, and let $H = -\Delta + V$ on $L^2(\mathbb{R}^3)$. Suppose that *either*:

(a) $\|V\|_R < 4\pi$;

or

(b) $Ve^{a|x|} \in R$ for some $a > 0$.

Then $\sigma_{\text{sing}}(H) = \varnothing$.

Proof (a) Since $\|V\|_R < 4\pi$, $|V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}$ has a Hilbert–Schmidt norm less than one uniformly for $\lambda \in \mathbb{C}\backslash[0, \infty)$ (see Section XI.6). Let $f \in C_0^\infty$ and note that $|f|^{1/2} \in R$. Then

$$\begin{aligned}|f|^{1/2}(H - \lambda)^{-1}|f|^{1/2} = {} & |f|^{1/2}(H_0 - \lambda)^{-1}|f|^{1/2} \\ & + \sum_{n=0}^{\infty} (-1)^{n+1} (|f|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}) \\ & \times (|V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2})^n \\ & \times (|V|^{1/2}(H_0 - \lambda)^{-1}|f|^{1/2})\end{aligned}$$

converges uniformly in Hilbert–Schmidt norm to an operator with norm less than $C_1 + C_2(1 - (4\pi)^{-1}\|V\|_R)^{-1}$. Thus

$$|(f, (H - \lambda)^{-1}f)| \leq \| |f|^{1/2} \|_2 \, \| |f|^{1/2}(H - \lambda)^{-1}|f|^{1/2} \|$$

is bounded on $\mathbb{C}\backslash[0, \infty)$. The fundamental criterion, Theorem XIII.19, thus implies that Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$ for *all* (a, b) so σ_{pp} and σ_{sing} are empty.

(b) As in our discussion in Section XI.6, $(1 + |V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2})^{-1}$ exists for all $\lambda \in \mathbb{C}\backslash[0, \infty)$ and has continuous boundary values as $\lambda \to x + i0$ as long as x avoids a finite set $\mathscr{E}$ of real numbers. Let $[a, b]$ be disjoint from $\mathscr{E}$. Then

$$\begin{aligned}|f|^{1/2}(H - \lambda)^{-1}|f|^{1/2} = {} & |f|^{1/2}(H_0 - \lambda)^{-1}|f|^{1/2} \\ & - (|f|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}) \\ & \times (1 + |V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2})^{-1}|V|^{1/2} \\ & \times (H_0 - \lambda)^{-1}|f|^{1/2}\end{aligned}$$

is a uniformly bounded operator on $\{x + i\varepsilon \,|\, 0 < \varepsilon < 1;\ x \in [a, b]\}$ whenever $f \in C_0^\infty$. As in (a), this implies that Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$ so $\sigma_{\text{sing}} \subset \mathscr{E}$, a finite set. This implies that $\sigma_{\text{sing}} = \varnothing$. ∎

Given the simple criterion, Theorem XIII.20, for $\sigma_{sing}(H)$ to be empty, one can reasonably ask why the problem of controlling the singular continuous spectrum is so much more difficult than that of identifying $\sigma_{ess}(H)$ (Sections 4 and 5) or $\sigma_{ac}(H)$ (Section XI.3). The reason is that σ_{sing} is much less stable under perturbations. To illustrate this, we describe the Aronszajn–Donoghue theory of the behavior of σ_{sing} under rank one perturbations. This theory should be compared with the Weyl theorem on invariance of σ_{ess} and the Kato–Birman theory of the invariance of σ_{ac}. Basic to the Aronszajn–Donoghue theory is the following combination of classical results of Fatou and de la Vallée Poussin:

Proposition Let ν be a finite Borel measure on $\mathbb{R}$ and let

$$F(z) = \int (x - z)^{-1}\, d\nu(x)$$

for $\operatorname{Im} z > 0$. Let $A_\nu = \{x \mid \lim_{\varepsilon \downarrow 0} F(x + i\varepsilon) = \infty\}$ and let

$$B_\nu = \{x \mid \lim_{\varepsilon \downarrow 0} F(x + i\varepsilon) = \Phi(x), \text{ a finite number with } \operatorname{Im} \Phi(x) \neq 0\}$$

Then $\nu(\mathbb{R} \setminus (A_\nu \cup B_\nu)) = 0$, $\nu \restriction A_\nu$ is singular relative to Lebesgue measure, and $\nu \restriction B_\nu$ is absolutely continuous.

Proofs of this result may be tracked down by consulting the reference in the notes. Now let H_0 be some self-adjoint operator on $\mathscr{H}$ and let $\varphi \in \mathscr{H}$ be a unit vector. Let P denote the projection onto φ and let

$$H_\alpha = H_0 + \alpha P$$

Let $\mathscr{H}'$ be the cyclic subspace for φ generated by H_0. Clearly all the H_α equal H_0 on $(\mathscr{H}')^\perp$ so we may as well suppose that $\mathscr{H}' = \mathscr{H}$, that is, we henceforth suppose that φ is cyclic for H_0. It follows that φ is also cyclic for H_α since

$$(H_\alpha - z)^{-1}\varphi = (H_0 - z)^{-1}\varphi - \alpha(\varphi, (H_0 - z)^{-1}\varphi)(H_\alpha - z)^{-1}\varphi$$

so that the span of $\{(H_\alpha - z)^{-1}\varphi\}$ is identical to the span of $\{(H_0 - z)^{-1}\varphi\}$. By this cyclicity result, H_α is unitarily equivalent to multiplication by x on $L^2(\mathbb{R}, d\nu_\alpha)$ for a suitable measure $d\nu_\alpha$.

Clearly,

$$F_\alpha(z) \equiv \int (x - z)^{-1}\, d\nu_\alpha(x) = (\varphi, (H_\alpha - z)^{-1}\varphi)$$

obeys

$$F_\alpha(z) = F_\beta(z) + (\beta - \alpha)F_\alpha(z)F_\beta(z)$$

on account of the resolvent equation

$$(H_\alpha - z)^{-1} = (H_\beta - z)^{-1} + (\beta - \alpha)(H_\alpha - z)^{-1}P(H_\beta - z)^{-1}$$

Thus, we have the basic equation:

$$F_\alpha(z) = F_\beta(z)(1 + (\alpha - \beta)F_\beta(z))^{-1} \tag{30.5}$$

Note that if $\lim_{\varepsilon \downarrow 0} F_\beta(z) = \infty$, then $\lim_{\varepsilon \downarrow 0} F_\alpha(z) = (\alpha - \beta)^{-1} \neq \infty$ for $\alpha \neq \beta$. Applying the proposition, we have proven the following striking *non-invariance* of σ_{sing}:

Theorem XIII.21.5 Let H_0 be a self-adjoint operator and let φ be a cyclic vector for H_0. Let

$$H_\alpha = H_0 + \alpha(\varphi, \cdot)\varphi$$

Then for $\alpha \neq \beta$ the singular (i.e., the union of pure point and singular continuous) parts of the spectral measures for H_α and H_β are mutually singular.

Example Let $d\nu_0 = dx \restriction [0, 1] + d\mu_C$, where $d\mu_C$ is the Cantor measure. Then $\sigma_{ess}(H_\alpha) = [0, 1]$ for all α on account of Weyl's theorem. Moreover, $F_0 = F_L + F_C$ in the obvious way, and

$$\lim_{\varepsilon \downarrow 0} \operatorname{Im} F_L(x + i\varepsilon) = \begin{cases} 1, & x \in (0, 1) \\ \frac{1}{2}, & x = 0, 1 \\ 0, & x \notin [0, 1] \end{cases}$$

Since $\operatorname{Im} F_C(z) \geq 0$ for all z with $\operatorname{Im} z > 0$, we see that $\lim_{\varepsilon \downarrow 0} F_0(x + i\varepsilon)$ is never real for any $x \in [0, 1]$. It follows from the basic equation (30.5) that $\lim_{\varepsilon \downarrow 0} F_\beta(x + i\varepsilon)$ is never infinite for $\beta \neq 0$, $x \in [0, 1]$. Thus, each H_β for $\beta \neq 0$ has no singular continuous spectrum while $\sigma_{sing}(H_0) \neq \varnothing$. Thus, we have two bounded operators H_0 and H_1 such that $H_0 - H_1$ has rank one, with $\sigma_{sing}(H_1) = \varnothing \neq \sigma_{sing}(H_0)$!

XIII.7 The absence of singular continuous spectrum II: Smooth perturbations

Theorem XIII.20 suggests that one study L^p bounds on expectation values of the resolvent and our experience suggests that $p = 2$ will be particularly easy to study.

Definition Let H be a self-adjoint operator with resolvent $R(\mu) = (H - \mu)^{-1}$. Let A be a closed operator. A is called ***H*-smooth** if and only if for each $\varphi \in \mathscr{H}$ and each $\varepsilon \neq 0$, $R(\lambda + i\varepsilon)\varphi \in D(A)$ for almost all $\lambda \in \mathbb{R}$ and moreover

$$\|A\|_H^2 = \sup_{\substack{\|\varphi\|=1 \\ \varepsilon>0}} \frac{1}{4\pi^2} \int_{-\infty}^{\infty} (\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2)\, d\lambda < \infty \quad (31)$$

Since A is closed, it is enough that (31) hold for a dense set of φ (Problem 47a). More interestingly, the uniform boundedness principle shows that if for *each* φ, $\int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2\, d\lambda \leq M_\varphi^2$ for a constant M_φ (independent of $\varepsilon > 0$ and of $\pm$, but dependent on φ), then A is H-smooth (Problem 47b,c).

The H-smooth operators are an especially nice class of operators. For example, we shall see that they are H-bounded with relative bound 0. They present in microcosm the close connection between scattering theory and spectral analysis. On one hand, we shall prove a basic result on the existence and completeness of wave operators $\Omega^{\pm}(H_1, H_0)$ when $H_1 - H_0$ is the product of an H_1-smooth operator and an H_0-smooth operator (Theorem XIII.24; see also Theorem XIII.31). On the other hand, we will see that if A is H-smooth, then $\overline{\text{Ran}(A^*)} \subset \mathscr{H}_{\text{ac}}(H)$ (Theorem XIII.23), which will lead to several theorems on the absence of singular continuous spectrum (see Theorems XIII.26 and XIII.28).

This section is divided into two parts. First, we shall develop the abstract theory of smooth perturbations, and in the second part we apply the theory to a variety of Schrödinger operators. The first two applications involve situations where the wave operators are unitary, i.e., where H and H_0 are unitarily equivalent. These are the cases of Schrödinger operators $H_0 + \lambda V$ with λ small or V repulsive. In the latter case, the theory of smooth perturbations will lead only to a proof that H has purely absolutely continuous spectrum. In our last application we shall establish the existence of wave operators for the case of repulsive potentials with some fall-off hypotheses by developing a generalization of the notion of H-smoothness. Part of this generalized theory will play a role in the next section.

One of our first main goals will be the reformulation of H-smoothness in a number of equivalent forms. We shall need the following vector-valued version of the Plancherel theorem.

Lemma 1 Let $\varphi(\cdot)$ be a (weakly measurable) function from $\mathbb{R}$ to a separable Hilbert space $\mathscr{H}$. Suppose that $\int \|\varphi(x)\|\, dx < \infty$. Define $\hat{\varphi}\colon \mathbb{R} \to \mathscr{H}$ by

$$\hat{\varphi}(p) = (2\pi)^{-1/2} \int_{\mathbb{R}} e^{-ipx}\varphi(x)\, dx$$

(where, by our standard convention, the integral is a weak integral). Let A be a closed operator on $\mathscr{H}$. Then

$$\int \|A\hat{\varphi}(p)\|^2\, dp = \int \|A\varphi(x)\|^2\, dx \quad (32)$$

where the integrals in (32) are set equal to ∞ if $\hat{\varphi}(p)$ (respectively, $\varphi(x)$) is not in $D(A)$ almost everywhere.

Proof First suppose that A is bounded. Then for any $\psi \in \mathscr{H}$, $(\psi, A\hat{\varphi}(p)) = (A^*\psi, \hat{\varphi}(p))$ is the (ordinary) Fourier transform of $(A^*\psi, \varphi(x)) = (\psi, A\varphi(x))$, so by the Plancherel theorem

$$\int |(\psi, A\hat{\varphi}(p))|^2\, dp = \int |(\psi, A\varphi(x))|^2\, dx$$

(32) follows by summing over ψ in an orthonormal basis. Next let A be self-adjoint and let $\{E_\Omega\}$ be its family of spectral projections. Then $AE_{(-a,a)}$ is bounded so

$$\int \|AE_{(-a,a)}\hat{\varphi}(p)\|^2\, dp = \int \|AE_{(-a,a)}\varphi(x)\|^2\, dx$$

Suppose that one of the integrals in (32) is finite—without loss suppose the right-hand side is finite. Then $\varphi(x) \in D(A)$ a.e. in x, so $\|AE_{(-a,a)}\varphi(x)\|^2$ converges monotonically to $\|A\varphi(x)\|^2$ as $a \to \infty$. Thus,

$$\int \lim_{a\to\infty} \|AE_{(-a,a)}\hat{\varphi}(p)\|^2\, dp = \int \|A\varphi(x)\|^2\, dx < \infty$$

In particular, $\lim_{a\to\infty} \|AE_{(-a,a)}\hat{\varphi}(p)\|^2 < \infty$ a.e. in p. It follows that $\hat{\varphi}(p) \in D(A)$ a.e. and (32) holds. Finally, let A be an arbitrary closed operator. By Theorem VIII.32, there is a self-adjoint operator $|A|$ with $D(|A|) = D(A)$ and $\||A|\psi\| = \|A\psi\|$. Thus (32) follows from the case where A is self-adjoint. ∎

Example 1 Let $H = -i\, d/dx$ on $L^2(\mathbb{R})$ so that $(e^{-iHt}\varphi)(x) = \varphi(x - t)$. Let g be in $L^2(\mathbb{R})$ and let A be multiplication by g. By a change of variables, $\int |g(x)\varphi(x - t)|^2\, dx\, dt = \|g\|_2^2\|\varphi\|_2^2$ so, by Fubini's theorem, for any $\varphi \in L^2$, and almost all t, $e^{-iHt}\varphi \in D(A)$ and $\int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2\, dt = \|g\|_2^2\|\varphi\|_2^2$. Fix $\varepsilon > 0$; then

$$\int_0^\infty e^{-\varepsilon t}e^{i\lambda t}e^{-iHt}\varphi\, dt = -iR(\lambda + i\varepsilon)\varphi$$

Thus, by the lemma

$$\int_{-\infty}^{\infty} \|AR(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = 2\pi \int_0^{\infty} e^{-2\varepsilon t} \|Ae^{-itH}\varphi\|^2 \, dt$$

Using a similar computation for $\lambda - i\varepsilon$, we see that

$$\int_{-\infty}^{\infty} (\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2) \, d\lambda = 2\pi \int_{-\infty}^{\infty} e^{-2\varepsilon|t|} \|Ae^{-itH}\varphi\|^2 \, dt \tag{33}$$

(33) and the bound on $\int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt$ imply that g is H-smooth and $\|g\|_H = (2\pi)^{-1/2}\|g\|_2$.

Example 2 Let H be any self-adjoint operator and let $A = I$, the identity operator. Again, we use Lemma 1 to conclude that

$$\int_{-\infty}^{\infty} \|R(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = 2\pi \int_0^{\infty} e^{-2\varepsilon t} \|e^{-itH}\varphi\|^2 \, dt = \pi\varepsilon^{-1}\|\varphi\|^2 \tag{34}$$

so that $\sup_{\varepsilon > 0} \int_{-\infty}^{\infty} \|R(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = \infty$ for any $\varphi \neq 0$. Thus I is never an H-smooth operator.

One reformulation of H-smoothness is in terms of the unitary group e^{itH}. As an immediate consequence of (33) we have:

Lemma 2 A is H-smooth if and only if for all $\varphi \in \mathscr{H}$, $e^{itH}\varphi \in D(A)$ for almost every $t \in \mathbb{R}$ and for some constant C,

$$\int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt \leq C\|\varphi\|^2$$

C can be chosen equal to $(2\pi)\|A\|_H^2$ and no smaller.

This lemma has several important consequences:

Theorem XIII.22 If A is H-smooth, then A is H-bounded with relative bound zero.

Proof Let $\psi \in D(A^*)$. By the resolvent formula

$$-i(A^*\psi, R(\lambda + i\varepsilon)\varphi) = \int_0^{\infty} (A^*\psi, e^{-iHt}\varphi)e^{i\lambda t}e^{-\varepsilon t} \, dt$$

Thus, by the Schwarz inequality

$$\begin{aligned} |(A^*\psi, R(\lambda + i\varepsilon)\varphi)|^2 &\leq \frac{1}{2\varepsilon} \int_0^{\infty} |(A^*\psi, e^{-iHt}\varphi)|^2 \, dt \\ &\leq \frac{1}{2\varepsilon} \|\psi\|^2 \int_0^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt \\ &\leq \frac{\pi}{\varepsilon} \|A\|_H^2 \|\psi\|^2 \|\varphi\|^2 \end{aligned}$$

by Lemma 2. Thus, $R(\lambda + i\varepsilon)\varphi \in D(A^{**}) = D(A)$ and $\|AR(\lambda + i\varepsilon)\|^2 \leq (\pi/\varepsilon)\|A\|_H^2$. We conclude that $D(H) \subset D(A)$ and for $\psi \in D(H)$

$$\|A\psi\| \leq \pi^{1/2}\|A\|_H(\varepsilon^{-1/2}\|H\psi\| + \varepsilon^{1/2}\|\psi\|)$$

Since ε is arbitrary, the theorem is proven. ∎

For a strengthening of Theorem XIII.22, see Problem 49.

Theorem XIII.23 If A is H-smooth, then $\overline{\mathrm{Ran}(A^*)} \subset \mathscr{H}_{\mathrm{ac}}(H)$.

Proof Since $\mathscr{H}_{\mathrm{ac}}(H)$ is closed, we need only show $\mathrm{Ran}(A^*) \subset \mathscr{H}_{\mathrm{ac}}(H)$. Let $\varphi \in D(A^*)$, $\psi = A^*\varphi$, and let $d\mu_\psi$ be the spectral measure for H associated with ψ. Define

$$F(t) = (2\pi)^{-1/2} \int e^{-itx} \, d\mu_\psi(x) = (2\pi)^{-1/2}(A^*\varphi, e^{-itH}\psi)$$

Then $|F(t)| \leq (2\pi)^{-1/2}\|\varphi\| \, \|Ae^{-itH}\psi\|$, so by Lemma 2, $F \in L^2(\mathbb{R})$. By the Plancherel theorem, $\check{F} \in L^2$ so $d\mu_\psi = \check{F} \, dx$ is absolutely continuous with respect to Lebesgue measure. ∎

It is an instructive exercise to prove Theorem XIII.23 using Theorem XIII.20 and the direct definition of H-smoothness. See also condition (5) of Theorem XIII.25 below. Lemma 2 has important consequences for scattering theory.

Theorem XIII.24 Let H and H_0 be self-adjoint operators. Suppose that $H = H_0 + \sum_{i=1}^n A_i^* B_i$ in the following sense:

(1) $D(H) \subset D(A_i)$; $D(H_0) \subset D(B_i)$; $i = 1, \ldots, n$.
(2) If $\varphi \in D(H)$ and $\psi \in D(H_0)$, then

$$(H\varphi, \psi) = (\varphi, H_0\psi) + \sum_{i=1}^n (A_i\varphi, B_i\psi) \tag{35}$$

Corollary If $AR(\mu)A^*$ is bounded for each $\mu \notin \mathbb{R}$ in the sense that

$$\sup_{\substack{\psi,\,\varphi \in D(A^*)\\ \|\psi\| = \|\varphi\| = 1}} |(A^*\varphi, R(\mu)A^*\psi)| < \infty \qquad \text{and} \qquad \Gamma \equiv \sup_{\mu \notin \mathbb{R}} \|AR(\mu)A^*\| < \infty$$

then A is H-smooth and $\|A\|_H \leq \Gamma/\pi$.

Proof of Theorem XIII.25 We first note that for every closed operator A, every bounded operator B, every $\varphi \in D(A)$, and $\psi \in \mathscr{H}$, we have

$$(\psi, BA\varphi) = (B^*\psi, A\varphi)$$

It follows that $\|BA\varphi\| \leq c\|\varphi\|$ for all $\varphi \in D(A)$ if and only if Ran $B^* \subset D(A^*)$ and $\|A^*B^*\| \leq c$. As a consequence $c_2 = c_3$ and $c_5 = c_6$. Moreover, since $(A^*\varphi, [R(\mu) - R(\bar{\mu})]A^*\varphi) = 2 \operatorname{Im} \mu \|R(\mu)A^*\varphi\|^2$, $c_5 = c_4$. Further, $c_0 = c_1$ by Lemma 2. Thus we need only prove that $c_0 = c_3 = c_4 = c_7$ where $c_0 \equiv \|A\|_H^2$. We shall show that

$$c_0 \leq c_4 \leq c_3 \leq c_0 \qquad \text{and} \qquad c_3 \leq c_7 \leq c_1 .$$

$c_0 \leq c_4$: $(2\pi i)^{-1}[R(\mu) - R(\bar{\mu})] = \pi^{-1}(\operatorname{Im} \mu)R(\bar{\mu})R(\mu) \geq 0$ if $\operatorname{Im} \mu > 0$. Let $K(\mu)$ be its positive square root. By the definition of c_4, $\|K(\mu)A^*\varphi\|^2 \leq c_4\|\varphi\|^2$ if $\varphi \in D(A^*)$. Thus, if $c_4 < \infty$, the remark above implies that Ran $K(\mu) \subset D(A)$ and $\|AK(\mu)\|^2 \leq c_4$. Therefore

$$\begin{aligned}
&\int_{-\infty}^{\infty} \|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi\|^2 \, d\lambda \\
&\quad = 4\pi^2 \int_{-\infty}^{\infty} \|AK(\lambda + i\varepsilon)K(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda \\
&\quad \leq 4\pi^2 c_4 \int_{-\infty}^{\infty} \|K(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda \\
&\quad = 4\pi^2 c_4 \frac{1}{2\pi i} \int_{-\infty}^{\infty} (\varphi, [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi) \, d\lambda \\
&\quad = 4\pi^2 c_4 \|\varphi\|^2
\end{aligned}$$

since in terms of the spectral measure $d\mu_\varphi$ for H,

$$\begin{aligned}
&(2\pi i)^{-1} \int_{-\infty}^{\infty} (\varphi, [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi) \, d\lambda \\
&\quad = \frac{\varepsilon}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{(x - \lambda)^2 + \varepsilon^2} \, d\mu_\varphi(x) \, d\lambda \\
&\quad = \int_{-\infty}^{\infty} d\mu_\varphi(x) = \|\varphi\|^2
\end{aligned}$$

Further,

$$[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi = i \int_{-\pi}^{\pi} e^{-\varepsilon|t|} e^{i\lambda t} e^{-iHt}\varphi \, dt$$

so Lemma 1 implies that

$$\int_{-\pi}^{\pi} \|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi\|^2 \, d\lambda = 2\pi \int_{-\infty}^{\pi} e^{-2\varepsilon|t|} \|Ae^{-iHt}\varphi\|^2 \, dt \quad (36)$$

so $c_0 = c_1 \leq c_4$.

$c_4 \leq c_3$: Let $\varphi \in D(A^*)$ and let $d\mu_{A^*\varphi}$ be the spectral measure for H with respect to $A^*\varphi$. Then, by (3)

$$d\mu_{A^*\varphi}(a, b] \leq c_3 |b - a| \, \|\varphi\|^2$$

If I is an arbitrary Borel set, let $|I|$ be its Lebesgue measure. It follows that $d\mu_{A^*\varphi}(I) \leq c_3 |I| \, \|\varphi\|^2$ for arbitrary I, for it is true for open sets and thus by outer regularity for arbitrary sets. Therefore $d\mu_{A^*\varphi}$ is absolutely continuous w.r.t. dx and the Radon–Nikodym derivative $g(x)$ obeys $\|g\|_\infty \leq c_3 \|\varphi\|^2$. Thus if $\mu = \lambda + i\varepsilon$, then

$$\begin{aligned}
|(A^*\varphi, [R(\mu) - R(\bar{\mu})]A^*\varphi)| &= \int_{-\infty}^{\infty} \frac{2|\varepsilon|}{(x - \lambda)^2 + \varepsilon^2} \, g(x) \, dx \\
&\leq \|g\|_\infty \int_{-\infty}^{\infty} \frac{2|\varepsilon|}{(x - \lambda)^2 + \varepsilon^2} \, dx \leq c_3(2\pi)\|\varphi\|^2
\end{aligned}$$

We conclude that $c_4 \leq c_3$.

$c_3 \leq c_0$: Let $\varphi \in D(A^*)$. Suppose that a and b are not eigenvalues of H. By Stone's formula,

$$\begin{aligned}
&|(A^*\varphi, E_{(a,b]}\psi)|^2 \\
&\quad = \frac{1}{4\pi^2} \lim_{\varepsilon \downarrow 0} \left| \int_a^b (A^*\varphi, [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\psi) \, d\lambda \right|^2 \\
&\quad \leq \frac{1}{4\pi^2} \|\varphi\|^2 \, |b - a| \lim_{\varepsilon \downarrow 0} \int_{-\infty}^{\infty} \|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\psi\|^2 \, d\lambda \\
&\quad \leq |b - a| \, \|A\|_H^2 \|\varphi\|^2 \, \|\psi\|^2
\end{aligned}$$

In the last step we have used (36). If a and/or b are eigenvalues, $a + \delta$ and $b + \delta$ are not eigenvalues for almost all small δ and $E_{(a,b]} = s\text{-}\lim_{\delta \to 0} E_{(a+\delta, b+\delta]}$ so we see that $c_3 \leq c_0$.

$c_3 \leq c_7$: We already know that $c_3 = c_6$, and $c_6 \leq c_7$ is obvious.

$c_7 \leq c_1$: This is essentially the argument used in the proof of Theorem XIII.22. For by that argument,

$$|(A^*\psi, R(\lambda + i\varepsilon)\varphi)|^2 \leq \frac{1}{2\varepsilon} \|\psi\|^2 \int_0^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt$$

so

$$\|AR(\lambda + i\varepsilon)\varphi\|^2 \leq \frac{1}{2\varepsilon}\int_0^\infty \|Ae^{-iHt}\varphi\|^2\, dt$$

A similar argument for $R(\lambda - i\varepsilon)$ proves that

$$\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2 \leq \frac{1}{2\varepsilon}\int_{-\infty}^\infty \|Ae^{-iHt}\varphi\|^2\, dt$$

Thus $c_7 \leq c_1$. ∎

Notice that criterion (3) provides another proof that $\mathrm{Ran}(A^*) \subset \mathscr{H}_{ac}(H)$ if A is H-smooth, and that criterion (6) implies Theorem XIII.22. The equality of c_6 and c_7 at first sight seems very mysterious. Some of this mystery can be removed by looking at the proof of a closely related equality:

$$\sup_{\substack{\varepsilon>0\\ \|\varphi\|=1}} \int_{-\infty}^\infty \|AR(\lambda + i\varepsilon)\varphi\|^2\, d\lambda = \sup_{\substack{\varepsilon>0\\ \|\varphi\|=1}} \left\{\int_{-\infty}^\infty (\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2)\, d\lambda\right\}$$

By (33), this equality is equivalent to

$$\sup_{\|\varphi\|=1} \int_0^\infty \|Ae^{-itH}\varphi\|^2\, dt = \sup_{\|\varphi\|=1} \int_{-\infty}^\infty \|Ae^{-itH}\varphi\|^2\, dt$$

which follows by noting that if $\varphi_s = e^{-isH}\varphi$, then

$$\int_0^\infty \|Ae^{-itH}\varphi_s\|^2\, dt = \int_s^\infty \|Ae^{-itH}\varphi\|^2\, dt$$

converges to $\int_{-\infty}^\infty \|Ae^{-itH}\varphi\|^2\, dt$ as $s \to -\infty$.

Before turning to applications, we give two more examples of smooth operators:

Example 3 Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and let A be multiplication by $V \in R$, the Rollnik class. By the estimate,

$$\begin{aligned}\||V|^{1/2}(H_0 - \lambda)^{-1}|V|^{1/2}\|_{\text{oper}} &\leq \||V|^{1/2}(H_0 - \lambda)^{-1}|V|^{1/2}\|_2 \\ &\leq (4\pi)^{-1}\|V\|_R\end{aligned}$$

and the corollary to Theorem XIII.25, $|A|^{1/2}$ is H-smooth.

Example 4 Let H be multiplication by x on $L^2([\alpha, \beta], dx)$ with $\alpha, \beta \in \mathbb{R}$. Let A be a bounded operator on $\mathscr{H}$ so that A^*A is an integral operator of the form

$$(A^*A\psi)(x) = \int_\alpha^\beta K(x, y)\psi(y)\, dy \tag{37}$$

with $\|K\|_\infty \equiv \operatorname{ess\,sup}_{[\alpha,\beta]\times[\alpha,\beta]} |K(x, y)| < \infty$. Then A is H-smooth with $\|A\|_H \leq \|K\|_\infty^{1/2}$. For, let $(a, b]$ be an interval and $\|\varphi\| = 1$. Then

$$\begin{aligned}\|AE(a, b]\varphi\|^2 &= (\varphi, E(a, b]A^*AE(a, b]\varphi) \\ &= \int_a^b \int_a^b K(x, y)\overline{\varphi(x)}\varphi(y)\, dx\, dy \\ &\leq \left(\int_a^b \int_a^b |K(x, y)|^2\, dx\, dy\right)^{1/2}\left(\int_a^b \int_a^b |\overline{\varphi}(x)\varphi(y)|^2\, dx\, dy\right)^{1/2} \\ &\leq |b - a|\,\|K\|_\infty\|\varphi\|^2\end{aligned}$$

By criterion (2), $\|A\|_H \leq \|K\|_\infty^{1/2}$. By further analysis (Problems 50, 51) one can show that for every H-smooth operator A, A^*A is of the form (37) and that $\|A\|_H = \|K\|_\infty^{1/2}$. In particular, we note that the analysis above shows that any integral operator

$$(A\psi)(x) = \int_\alpha^\beta A(x, y)\psi(y)\, dy$$

with $\|A\|_\infty < \infty$ is H-smooth. We have thus found many H-smooth operators and, in particular, H-smooth operators A with $\mathrm{Ker}(A) = \{0\}$. Example 1 is related to this example although the operator H in Example 1 is not bounded. For if $f \in L^2$, then $A =$ multiplication by f has $A^*A =$ multiplication by $g \equiv |f|^2 \in L^1$. Passing to the representation in which $-i\, d/dx$ is diagonal (by using Fourier transform), A^*A is an integral operator with kernel equal to $(2\pi)^{-1/2}\hat{g}(x - y) \in L^\infty$.

We turn now to various applications:

A. Weakly coupled quantum systems

Suppose that H_0 is a positive self-adjoint operator and that C is self-adjoint. If $|C|^{1/2}(H_0 + I)^{-1}|C|^{1/2}$ is a bounded operator with bound a, then for any $\varphi \in D(|C|^{1/2})$, $\|(H_0 + I)^{-1/2}|C|^{1/2}\varphi\|^2 \leq a\|\varphi\|^2$ so

$(H_0 + I)^{-1/2}|C|^{1/2}$ is bounded. Taking adjoints, $Q(H_0) \subset Q(C)$ and $\||C|^{1/2}(H_0 + I)^{-1/2}\|^2 \leq a$. It follows that $(\varphi, |C|\varphi) \leq a(\varphi, (H_0 + I)\varphi)$ for all $\varphi \in Q(H_0)$. Thus C is H_0-form bounded and if $a < 1$, the form sum $H = H_0 + C$ is self-adjoint. Such form sums are the subject of the following theorem.

Theorem XIII.26 (Kato's smoothness theorem) Let H_0 be a positive self-adjoint operator on a Hilbert space $\mathscr{H}$ and let $C_1, \ldots, C_n$ be self-adjoint operators with

$$\alpha_{ij} \equiv \sup_{\mu \notin \mathbb{R}} \| |C_i|^{1/2}(H_0 - \mu)^{-1}|C_j|^{1/2}\| < \infty$$

Suppose that $\{\alpha_{ij}\}_{1 \leq i, j \leq n}$ is the matrix of an operator of norm less than 1 on $\mathbb{C}^n$ (with the natural Hilbert space norm). Then:

(a) The form sum $H = H_0 + \sum_{i=1}^n C_i$ is a closed form on $Q(H_0)$.
(b) The wave operators $\text{s-lim}_{t \to \mp\infty} e^{iHt}e^{-iH_0t}$ exist and are unitary.

In particular, H and H_0 are unitarily equivalent operators.

Proof Introduce the Hilbert space $\mathscr{H}' = \oplus_{i=1}^n \mathscr{H}_i$ where each $\mathscr{H}_i$ is a copy of $\mathscr{H}$. By the discussion preceding the theorem and the hypothesis $\alpha_{ii} < \infty$, we have that each $|C_i|$ is H_0-form bounded, so that $|C_i|^{1/2}$ is defined from $Q(H_0)$ to $\mathscr{H}$. As a result, we can define B: $Q(H_0) \to \mathscr{H}'$ by $(B\psi)_i = |C_i|^{1/2}\psi$. The hypothesis of the theorem implies that

$$\alpha \equiv \sup_{\mu \notin \mathbb{R}} \| B(H_0 - \mu)^{-1}B^* \| < 1 \tag{38}$$

Let $B = U|B|$ be the polar decomposition of B. Then, since $|B| = U^*B$ and U is a partial isometry, (38) implies that $|B|(H_0 + I)^{-1}|B|$ is a bounded operator of norm smaller than α. Again, it follows from the argument preceding the theorem that

$$(\varphi, |B|^2\varphi) \leq \alpha(\varphi, (H_0 + I)\varphi)$$

or that

$$\left(\varphi, \sum_{i=1}^n |C_i|\varphi\right) \leq \alpha(\varphi, (H_0 + I)\varphi) \tag{39}$$

From (39), we conclude that $\sum_{i=1}^n C_i$ is H_0-form bounded with relative bound $\alpha < 1$ proving (a).

Next, we note that for $\mu \notin [0, \infty)$,

$$(H - \mu)^{-1} = (H_0 - \mu)^{-1} - \sum_{n=0}^{\infty}(-1)^n(H_0 - \mu)^{-1}B^*W(B(H_0 - \mu)^{-1}B^*W)^nB(H_0 - \mu)^{-1} \tag{40}$$

where W: $\mathscr{H}' \to \mathscr{H}'$ by $(W\varphi)_i = (\text{sgn } C_i)\varphi_i$. (40) holds since the sum is convergent by (38) and one checks that, in the language of quadratic forms (Section VIII.6), the right-hand side maps $\mathscr{H}_{-1}$ to $\mathscr{H}_{+1}$ and is an inverse for $(H - \mu)$: $\mathscr{H}_{+1} \to \mathscr{H}_{-1}$. From (40) one easily sees that

$$\sup_{\mu \notin \mathbb{R}} \|B(H - \mu)^{-1}B^*\| \leq \alpha(1 - \alpha)^{-1} \tag{41}$$

so each $|C_i|^{1/2}$ and $C_i^{1/2} \equiv |C_i|^{1/2}\,\text{sgn } C_i$ is H-smooth by the corollary to Theorem XIII.25. Similarly, by the basic hypotheses and that corollary, each $|C_i|^{1/2}$ is H_0-smooth. Thus, by Theorem XIII.24, both $\text{s-lim}_{t \to \mp\infty} e^{iHt}e^{-iH_0t}$ and $\text{s-lim}_{t \to \mp\infty} e^{iH_0t}e^{-iHt}$ exist. These maps are all isometries and inverses of one another. This proves (b). ∎

As an application of this theorem, the reader should prove the strong version of Theorem XIII.21 found in Problem 56. If one does not want to worry about detailed estimates, it is often useful to state Kato's smoothness theorem in the form:

Corollary Let H_0 be self-adjoint and positive. Let $C_1, \ldots, C_n$ be self-adjoint and let $C = \sum_{i=1}^n C_i$. Suppose that for each i and j

$$\sup_{\mu \notin \mathbb{R}} \| |C_i|^{1/2}(H_0 - \mu)^{-1}|C_j|^{1/2}\| < \infty$$

Then there exists $\Lambda > 0$ so that for all $\lambda \in (-\Lambda, \Lambda)$:

(a) $H(\lambda) = H_0 + \lambda C$ is a closed form on $Q(H_0)$.
(b) The wave operators $\Omega_\lambda^\pm = \text{s-lim}_{t \to \mp\infty} e^{itH(\lambda)}e^{-itH_0}$ exist and are unitary.

It is actually possible to prove that $\Omega_\lambda^\pm$ are analytic in λ (see the Notes and Problems 53, 54). Now we can easily handle "weakly coupled" N-body Schrödinger operators.

Theorem XIII.27 (the Iorio–O'Carroll theorem) Let $m \geq 3$, $N \geq 2$. Let $\tilde{H}_0$ be the operator

$$\tilde{H}_0 = \sum_{i=1}^{N} (-2\mu_i)^{-1} \Delta_i$$

on $L^2(\mathbb{R}^{Nm})$ where each $\mu_i > 0$ and $r \in \mathbb{R}^{Nm}$ is written $r = \langle r_1, \ldots, r_N \rangle$ with $r_i \in \mathbb{R}^m$. Let H_0 be $\tilde{H}_0$ with the center of mass motion removed (see Section XI.5). Let $V = \sum_{i<j} V_{ij}(r_i - r_j)$ where each $V_{ij} \in L^{m/2+\varepsilon}(\mathbb{R}^m) \cap L^{m/2-\varepsilon}(\mathbb{R}^m)$ for some fixed $\varepsilon > 0$. Then for all $\lambda \in \mathbb{R}$ with $|\lambda|$ sufficiently small, $H_0 + \lambda V$ (defined as a form sum) is unitarily equivalent to H_0. The wave operators provide unitary equivalence. In particular, $H_0 + \lambda V$ has no bound states, no singular spectrum and has complete scattering.

Before proving the Iorio–O'Carroll theorem, we make several remarks. First, it is merely for contact with the notions of N-body quantum theory that we remove the center of mass motion. Secondly, we note that only when $m = 3$ is the form sum necessary. If $m \geq 4$, Theorem X.20 tells us that the operator sum $H_0 + \lambda V$ is self-adjoint on $C_0^\infty(\mathbb{R}m(N-1)$ if λ is real. Thirdly, we note that, by Theorem XIII.11, there can be no weak coupling theorem when $m = 1$ or 2, but there is a result on $L^2([0, \infty))$ (Problem 58). Finally, the conditions on V_{ij} cannot be weakened much; for if V_{ij} has non-$L^{m/2}$ local singularities at finite points (e.g., $r^{-2-\varepsilon}$ behavior at $r = 0$), then self-adjointness is lost and if V_{ij} has non-$L^{m/2}$ behavior at infinity (e.g., only $r^{-2+\varepsilon}$ falloff at ∞), then it can happen that $H_0 + \lambda V$ has bound states no matter how small λ is (see Theorem XIII.6).

Proof of Theorem XIII.27 Consider first the case $N = 2$. Then $H_0 = (-2\nu)^{-1} \Delta$ on $L^2(\mathbb{R}^m)$, so by Theorem IX.30,

$$\|e^{-iH_0 t}\varphi\|_r \leq (ct)^{-m[\frac{1}{2}-r^{-1}]}\|\varphi\|_{r'} \tag{42}$$

where $2 \leq r \leq \infty$, $r^{-1} + r'^{-1} = 1$ and c is chosen suitably. Thus, if $f \in L^p$ and $p > 2$, then by Hölder's inequality and (42)

$$\|fe^{-iH_0 t}f\varphi\|_2 \leq (ct)^{-mp^{-1}}\|f\|_p^2\|\varphi\|_2 \tag{43}$$

Thus, if $f \in L^{m-\varepsilon} \cap L^{m+\varepsilon}$ (and $m > 2 + \varepsilon$),

$$\int_{-\infty}^{\infty} \|fe^{-iH_0 t}f\varphi\|_2 \, dt \leq d(\|f\|_{m+\varepsilon} + \|f\|_{m-\varepsilon})^2\|\varphi\|_2$$

for a suitable constant d. Since

$$f(H_0 - z)^{-1}f\varphi = i\int_0^\infty e^{izt}(fe^{-iH_0 t}f)\varphi \, dt$$

if $\operatorname{Im} z > 0$, we conclude that

$$\|f(H_0 - z)^{-1}f\varphi\|_2 \leq d(\|f\|_{m+\varepsilon} + \|f\|_{m-\varepsilon})^2\|\varphi\|_2$$

if $\operatorname{Im} z > 0$. A similar argument holds if $\operatorname{Im} z < 0$. Letting $f = |V|^{1/2}$, we conclude that

$$\sup_{z \notin \mathbb{R}} \| \, |V|^{1/2}(H_0 - z)^{-1}|V|^{1/2}\| < \infty$$

The theorem (in case $N = 2$) then follows from the corollary to Theorem XIII.26.

To prove the theorem in the general case, we need only prove that

$$\sup_{z \notin \mathbb{R}} \| \, |V_{ij}|^{1/2}(H_0 - z)^{-1}|V_{k\ell}|^{1/2}\| < \infty$$

for all i, j, k, ℓ and apply the corollary to Theorem XIII.26. It is necessary to consider three distinct cases:

Case 1 $(ij) = (k\ell)$ Without loss of generality suppose that $i = k = 1$ and $j = \ell = 2$. Let $H_0^{(12)} = (-2\mu_{12})^{-1} \Delta_{12}$ where $\mu_{12}^{-1} = \mu_1^{-1} + \mu_2^{-1}$ and Δ_{12} is the Laplacian with respect to r_{12} in a Jacobi coordinate system (see Section XI.5). Thus, $H_0 - H_0^{(12)}$ depends only on the remaining Jacobi coordinates $\zeta_2, \ldots, \zeta_{N-1}$ and so commutes with any function of $\zeta_1 = r_2 - r_1$. If $f \in L^p(\mathbb{R}^m)$ and f_1 is multiplication by $f(\zeta_1)$, then

$$\|f_1 e^{-itH_0}f_1\varphi\|_2 = \|f_1 e^{-itH_0^{(12)}}f_1\varphi\|_2 \tag{44}$$

Let $\varphi \in \mathscr{S}(\mathbb{R}^{m(N-1)})$. By the basic two-body estimate (43),

$$\int |f_1(e^{-iH_0^{(12)}t}f_1\varphi(\zeta_1, \zeta_2, \ldots, \zeta_{N-1})|^2 \, d\zeta_1 \leq (ct)^{-2mp^{-1}}\|f\|_p^4 \int |\varphi(\zeta)|^2 \, d\zeta_1$$

Integrating over $\zeta_2, \ldots, \zeta_{N-1}$ and using (44) we see that (43) still holds. Thus, by mimicking the two-body proof,

$$\sup_{z \notin \mathbb{R}} \| \, |V_{12}|^{1/2}(H_0 - z)^{-1}|V_{12}|^{1/2}\| < \infty$$

Case 2 $j = k$; i, j, ℓ distinct Without loss of generality, suppose that $i = 1$; $j = k = 2$; $\ell = 3$. Again use Jacobi coordinates with $\zeta_1 = r_2 - r_1$ and with $r_{23} = \alpha\zeta_1 + \beta\zeta_2$ (with $\alpha, \beta \neq 0$). Since $H_0 - H_0^{(12)}$ commutes with functions of ζ_1:

$$\| \, |V_{12}|^{1/2}e^{-itH_0}|V_{23}|^{1/2}\varphi\| = \| \, |V_{12}|^{1/2}e^{-itH_0^{(12)}}|V_{23}|^{1/2}\varphi\|$$

Fix $\zeta' \equiv \langle \zeta_2, \ldots, \zeta_{N-1} \rangle$ and let $\varphi \in \mathscr{S}(\mathbb{R}^{m(N-1)})$. Then by the basic two-body estimate (43),

$$\int |V_{12}(\zeta_1)|\, |e^{-itH_0^{(12)}} V_{23}^{1/2}(\alpha\zeta_1 - \beta\zeta_2)\varphi(\zeta_1, \zeta')|^2 \, d\zeta_1$$

$$\leq (ct)^{-2mp^{-1}} \|V_{12}\|_{p/2} \|V_{23}\|_{p/2} \alpha^{-2m/p} \int |\varphi(\zeta)|^2 \, d\zeta_1$$

where we have used the fact that

$$\int |V_{23}(\alpha\zeta_1 - \beta\zeta_2)|^{p/2} \, d\zeta_1 = \alpha^{-1} \int |V_{23}(x)|^{p/2} \, dx$$

independently of ζ_2. Integrating over ζ', we find that

$$\| |V_{12}|^{1/2} e^{-itH_0^{(12)}} |V_{23}|^{1/2} \varphi \|_2^2 \leq \alpha^{-2/p} (ct)^{-2mp^{-1}} \|V_{12}\|_{p/2} \|V_{23}\|_{p/2} \|\varphi\|_2^2$$

From this estimate, it follows that

$$\sup_{z \notin \mathbb{R}} \| |V_{12}|^{1/2} (H_0 - z)^{-1} |V_{23}|^{1/2} \| < \infty$$

as in the two-body case.

Case 3 *i, j, k, ℓ all distinct* Without loss of generality suppose that $i = 1, j = 2, k = 3, \ell = 4$. Then,

$$\begin{aligned} &|(\varphi, |V_{12}|^{1/2} e^{-itH_0} |V_{34}|^{1/2} \psi)| \\ &\quad = |(e^{+itH_0^{(34)}} \varphi, |V_{12}|^{1/2} e^{-it(H_0 - H_0^{(34)})} |V_{34}|^{1/2} \psi)| \\ &\quad = |(|V_{34}|^{1/2} e^{itH_0^{(34)}} \varphi, |V_{12}|^{1/2} e^{-it(H_0 - H_0^{(34)})} \psi)| \\ &\quad \leq \| |V_{34}|^{1/2} e^{itH_0^{(34)}} \varphi \| \, \| |V_{12}|^{1/2} e^{-itH_0^{(12)}} \psi \| \end{aligned}$$

In the first step, we have used the fact that $|V_{12}|^{1/2}$ and $H_0^{(34)}$ commute; in the second step that $|V_{34}|^{1/2}$ commutes with $H_0 - H_0^{(34)}$ and $|V_{12}|^{1/2}$; and in the final step that $|V_{12}|^{1/2}$ and $H_0 - H_0^{(34)} - H_0^{(12)}$ commute. By step (1) and the corollary to Theorem XIII.25, $|V_{ij}|^{1/2}$ is $H_0^{(ij)}$-smooth. Thus,

$$\begin{aligned} &\int_{-\infty}^{\infty} \| |V_{34}|^{1/2} e^{+itH_0^{(34)}} \varphi \| \, \| |V_{12}|^{1/2} e^{-itH_0^{(12)}} \psi \| \, dt \\ &\quad \leq \left(\int_{-\infty}^{\infty} \| |V_{34}|^{1/2} e^{itH_0^{(34)}} \varphi \|^2 \, dt \right)^{1/2} \\ &\quad \times \left(\int_{-\infty}^{\infty} \| |V_{12}|^{1/2} e^{-itH_0^{(12)}} \psi \|^2 \, dt \right)^{1/2} \\ &\quad \leq \| |V_{34}|^{1/2} \|_{H_0^{(34)}} \, \| |V_{12}|^{1/2} \|_{H_0^{(12)}} \, \|\varphi\| \, \|\psi\| \end{aligned}$$

so that

$$\int_{-\infty}^{\infty} |(\varphi, |V_{12}|^{1/2} e^{-itH_0} |V_{34}|^{1/2} \psi)| \, dt \leq c \|\varphi\| \, \|\psi\|$$

Since

$$\begin{aligned} &(\varphi, |V_{12}|^{1/2} (H_0 - z)^{-1} |V_{34}|^{1/2} \psi) \\ &\quad = -i \int_0^{\infty} e^{izt} (\varphi, |V_{12}|^{1/2} e^{-iH_0 t} |V_{23}|^{1/2} \psi) \, dt \end{aligned}$$

if $\operatorname{Im} z > 0$, we conclude that

$$\sup_{z \notin \mathbb{R}} \| |V_{12}|^{1/2} (H_0 - z)^{-1} |V_{34}|^{1/2} \| < \infty$$

This completes the proof of case 3. ∎

If one of the particles has infinite mass, Case 2 cannot be handled as above since $\alpha = 0$ if $\mu_2 = \infty$. In that event, the method of case 3 will work and the theorem remains true.

B. Positive commutators and repulsive potentials

As a second application of smoothness techniques, we develop a method that will allow us to prove that Hamiltonians with repulsive potentials have purely absolutely continuous spectrum.

Theorem XIII.28 (the Putnam–Kato theorem) Let H and A be bounded self-adjoint operators. Suppose that $C = i[H, A]$ is positive. Then $C^{1/2}$ is H-smooth. In particular, if $\operatorname{Ker} C = \{0\}$, then H has purely absolutely continuous spectrum.

Proof The second statement follows from the first by Theorem XIII.23 and the fact that $\operatorname{Ker}(C^{1/2}) = [\operatorname{Ran}(C^{1/2})]^{\perp} = \{0\}$. We compute:

$$\frac{d}{dt} e^{itH} A e^{-itH} \varphi = i e^{itH} [H, A] e^{-itH} \varphi = e^{itH} C e^{-itH} \varphi$$

Thus

$$\int_s^t (\varphi, e^{i\tau H} C e^{-i\tau H} \varphi) \, d\tau = (\varphi, e^{itH} A e^{-itH} \varphi) - (\varphi, e^{isH} A e^{-isH} \varphi)$$

so

$$\int_s^t \|C^{1/2}e^{-itH}\varphi\|^2\, d\tau \leq 2\|A\|\,\|\varphi\|^2$$

Since t and s are arbitrary, $C^{1/2}$ is H-smooth and

$$\|C^{1/2}\|_H^2 \leq \|A\|/\pi \quad \blacksquare$$

For an alternative method of proof, see Problem 59.

Example 5 Since examples of positive commutators are not easy to construct directly, we present examples to show that the hypotheses of Theorem XIII.28 are sometimes obeyed. In fact, there is a sort of converse to the fact that $C^{1/2}$ is H-smooth: If H is bounded and B is any bounded H-smooth operator, there exists a bounded operator A with $i[H, A] = B^*B$. Since there are H-smooth operators with zero kernel when H has purely absolutely continuous spectrum (see Example 4), one can construct many pairs H, A for which the hypotheses of Theorem XIII.28 are obeyed. If B is H-smooth, then by following the argument in Theorem XIII.24, one can show that $\Gamma_H^+(B^*B) \equiv \text{s-lim}_{s\to\infty}\, i\int_0^s e^{itH}B^*Be^{-itH}\,dt$ exists. Now,

$$\begin{aligned}[H, \Gamma_H^+(B^*B)] &= \text{s-lim}_{s\to\infty}\, i\int_0^s e^{itH}[H, B^*B]e^{-itH}\,dt \\ &= \text{s-lim}_{s\to\infty}\,(e^{isH}B^*Be^{-isH} - B^*B) \\ &= -B^*B\end{aligned}$$

where we have used the fact that $e^{itH}B^*Be^{-itH}\varphi \in L^2$ with a uniformly bounded derivative to conclude that $\text{s-lim}_{s\to\infty}\,(e^{isH}B^*Be^{-isH}) = 0$ (Problem 62). Letting $A = i\Gamma_H^+(B^*B)$, we see that $i[H, A] = B^*B$.

We want to apply the idea of positive commutators to prove that N-body Schrödinger operators with repulsive potentials have purely absolutely continuous spectrum. A repulsive potential is a function on $\mathbb{R}^m$ so that $V(r\hat{e}) \leq V(r'\hat{e})$ for each unit vector $\hat{e}$ and all $r > r'$. Thus repulsive potentials tend to push particles apart, so we expect no bound states and thus only absolutely continuous spectra. There is another way of describing the fact that V is repulsive that makes the connection with positive commutators clearer. Let $U(\theta)$ be the family of dilations, $(U(\theta)\psi)(r) = e^{+m\theta/2}\psi(e^\theta r)$. Then $[U(\theta)VU(\theta)^{-1}](r) = V(e^\theta r)$, so repulsive potentials obey the condition

that $V_\theta \equiv U(\theta)VU(\theta)^{-1}$ is monotone decreasing as θ increases. Since $U(\theta)H_0\,U(\theta)^{-1} = e^{-2\theta}H_0$, the kinetic energy also decreases monotonically under dilations. Thus, formally,

$$\frac{d}{d\theta}\,U(\theta)(H_0 + V)U(\theta)^{-1} \leq 0$$

Letting

$$D = \frac{i}{2}\sum_{i=1}^m \left(x_i\frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_i}x_i\right)$$

be the generator of $U(\theta)$ (i.e., $U(\theta) = \exp(-i\theta D)$), we see that $i[D, H] \geq 0$ formally.

Physically, there is another way of looking at the fact that $i[D, H] \geq 0$. For $D = -(i/2)[H, x^2]$. Therefore, if one defines the Heisenberg picture moment of inertia

$$I(t) = e^{+iHt}x^2e^{-iHt}$$

then on a formal level $i[D, H] \geq 0$ is equivalent to $\ddot{I}(t) \geq 0$. It is easy to see that classically the repulsive potential obeys this condition and indeed we have used similar ideas in Theorem XI.3.

Theorem XIII.28 is not directly applicable for three reasons: (1) The computations were formal; as usual this requires care with domains and cores, but it turns out that no extra technical assumption is needed. (2) H is not bounded. It turns out that since H is positive, this in itself would not be very serious (see Problem 61). (3) D is not bounded. This is more serious. The d/dx piece of D is not hard to control since it is H-bounded but the factor of x is hard to control directly. In the proof of the theorem below, we will use a cutoff x which will have the effect of making the computations more complicated. Since V being repulsive is related to $dV/dr \leq 0$, it is the derivative in D rather than the x that is important—thus cutting off x will not destroy $i[A, H] \geq 0$.

Theorem XIII.29 (Lavine's theorem) Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^m)$ $(m \geq 3)$. Let V be a function on $\mathbb{R}^m$ so that

(i) Multiplication by V is H_0-bounded with relative bound zero.
(ii) The distributional derivative $\sum_{i=1}^n x_i\,\partial V/\partial x_i$ is negative.

Then $H = H_0 + V$ has purely absolutely continuous spectrum.

Proof Choose α obeying $\frac{1}{2} < \alpha < \frac{3}{2}$ and define $g(r) = \int_0^r (1+\rho^2)^{-\alpha}\, d\rho$. Let A be the operator

$$Af = i \sum_{k=1}^{m} \left[x_k \frac{g(r)}{r} \frac{\partial f}{\partial x_k} + \frac{\partial}{\partial x_k}\left(x_k \frac{g(r) f}{r} \right) \right] \tag{45}$$

Since $g(r)r^{-1}$ is C^∞, A maps C_0^∞ into itself. If g were replaced by r in (45), the operator resulting would be the generator of dilations, so (45) is a partially cutoff version of this generator. In fact, A has a direct geometrical interpretation. Let $T_\gamma\colon \mathbb{R}^n \to \mathbb{R}^n$ be defined by the conditions: $T_0(x) = x$, and $y(\gamma) = T_\gamma x$ solves $\dot{y} = |y|^{-1} g(|y|) y$. Then,

$$(e^{-i\gamma A} f)(x) = N_\gamma(x) f(T_\gamma x)$$

where $N_\gamma(x)$ is a normalizing factor (the square root of a Jacobian determinant).

Our first goal is to prove that for some constant $c > 0$,

$$i[A, H] \geq c(1+r^2)^{-\alpha-1}$$

in the sense that for all $\varphi \in C_0^\infty(\mathbb{R}^n)$,

$$i(A\varphi, H\varphi) - i(H\varphi, A\varphi) \geq c(\varphi, (1+r^2)^{-\alpha-1}\varphi) \tag{46}$$

First, we compute

$$\begin{aligned} &i(A\varphi, V\varphi) - i(V\varphi, A\varphi) \\ &\quad = 2\,\mathrm{Re} \sum_{i=1}^{m} \int V(x) \left[\overline{\varphi(x)} \left\{ \frac{x_i}{r} g(r) \frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\frac{x_i}{r} g(r) \right) \right\} \varphi(x) \right] dx \\ &\quad = 2 \int V(x) \sum_{i=1}^{m} \frac{\partial}{\partial x_i} x_i \left(\frac{g(r)}{r} |\varphi(x)|^2 \right) dx \geq 0 \end{aligned}$$

by hypothesis (ii). Thus we need only verify (46) when $V = 0$, a tedious but not too difficult task. As a preliminary, we note that for all r,

$$rg'(r) - g(r) \leq 0 \tag{47a}$$

$$g''(r) = -2\alpha r(1+r^2)^{-\alpha-1} \tag{47b}$$

$$g'''(r) + (2\alpha+1) r^{-1} g''(r) \leq 0 \tag{47c}$$

To prove (47a), we remark that $(1+r^2)^{-\alpha}$ is monotone decreasing, so its average value $g(r)r^{-1} = r^{-1}\int_0^r (1+\rho^2)^{-\alpha}\, d\rho$ is also monotone decreasing. Since $rg' - g = r^2(r^{-1}g)'$, (47a) is proven. (47b) and (47c) follow from the explicit calculations:

$$g''(r) = -2\alpha r(1+r^2)^{-\alpha-1}$$

$$g'''(r) + (2\alpha+1) r^{-1} g''(r) = -4\alpha(\alpha+1)(1+r^2)^{-\alpha-2}$$

Next we prove that

$$-\Delta\left(\sum_{j=1}^{m} \frac{\partial g_j}{\partial x_j} \right) \geq c(1+r^2)^{-\alpha-1} \tag{48}$$

where $g_j(x) = x_j r^{-1} g(r)$. For

$$\frac{\partial g_j}{\partial x_k} = r^{-1} g(\delta_{jk} - r^{-2} x_j x_k) + r^{-2} x_j x_k g' \tag{49}$$

Thus

$$\sum_{j=1}^{m} \frac{\partial g_j}{\partial x_j} = (n-1) r^{-1} g + g'$$

Using the fact that for a spherically symmetric function h,

$$\Delta h = r^{-1}(rh)'' + (n-3) r^{-1} h'$$

we find that

$$\begin{aligned} -\Delta\left(\sum_{j=1}^{n} \frac{\partial g_j}{\partial x_j} \right) &= -(g''' + (2\alpha+1) r^{-1} g'') - (2n - 2\alpha - 3) r^{-1} g'' \\ &\quad - (n-1)(n-3) r^{-3}(rg' - g) \end{aligned}$$

Since $n \geq 3$ and $\alpha < \frac{3}{2}$, (48) follows from (47). Finally, we compute on C_0^∞ functions that

$$\begin{aligned} -\left[g_k \frac{\partial}{\partial x_k}, H_0 \right] &= \sum_{i=1}^{n} \left[g_k \frac{\partial}{\partial x_k}, \frac{\partial^2}{\partial x_i^2} \right] \\ &= \sum_{i=1}^{n} 2p_i \frac{\partial g_k}{\partial x_i} p_k + i \frac{\partial^2 g_k}{\partial x_i^2} p_k \end{aligned}$$

where $p_k = i^{-1}\, \partial/\partial x_k$. Using

$$-\left[g_k \frac{\partial}{\partial x_k} + \frac{\partial}{\partial x_k} g_k, H_0 \right] = -\left[g_k \frac{\partial}{\partial x_k}, H_0 \right] - \left[g_k \frac{\partial}{\partial x_k}, H_0 \right]^*$$

we see that

$$i[A, H_0] = \sum_{i,k} 2p_k \left(\frac{\partial g_i}{\partial x_k} + \frac{\partial g_k}{\partial x_i} \right) p_i - \Delta\left(\sum_j \frac{\partial g_j}{\partial x_j} \right)$$

Thus by (48) the proof of (46) has been reduced to proving

$$\sum_{i,k} 2p_k \left(\frac{\partial g_i}{\partial x_k} + \frac{\partial g_k}{\partial x_i} \right) p_i \geq 0 \tag{50}$$

By (49) the left-hand side of (50) is

$$4\sum_{i,k}\{p_k[(r^{-1}g)(\delta_{ik}-r^{-2}x_ix_k)]p_i+p_k(r^{-2}g')x_ix_kp_i\}$$

Fix $x\in\mathbb{R}^n$. Then, by the Schwarz inequality, the matrix $\{\delta_{ik}-r^{-2}x_ix_k\}$ is positive definite. Further, $\{x_ix_kr^{-2}\}$ is clearly positive definite, so (50) holds and this completes the proof of (46).

Next, we need to know that $A<<H$, i.e., that A is H-bounded with relative bound zero. Since $V<<H_0$ by hypothesis, we need only prove that $A<<H_0$. But $\partial/\partial x_i<<H_0$, x_igr^{-1} is bounded, and

$$A=2i\sum_{i=1}^{n}x_igr^{-1}\,\partial/\partial x_i+i(n-1)r^{-1}g+ig'$$

so $A<<H_0$ is proven. Since C_0^∞ is a core for H and $A<<H$, (46) holds for all $\varphi\in D(H)$.

Now let $\varphi\in D(H)$ and let B be multiplication by $c^{1/2}(1+r^2)^{-(\alpha+1)/2}$. Then we claim that

$$\int_{-\infty}^{\infty}\|Be^{-itH}\varphi\|^2\,dt\le d\|(H+I)\varphi\|^2 \tag{51}$$

for a suitable constant d. For, by (46),

$$\begin{aligned}&\int_{-\infty}^{\infty}\|Be^{-itH}\varphi\|^2\,dt\\&\quad=\int_{-\infty}^{\infty}(e^{-itH}\varphi,\,B^*Be^{-itH}\varphi)\,dt\\&\quad\le\int_{-\infty}^{\infty}i\{(Ae^{-itH}\varphi,\,He^{-itH}\varphi)-(He^{-itH}\varphi,\,Ae^{-itH}\varphi)\}\,dt\\&\quad\le 2\sup_{-\infty<s<\infty}|(e^{-isH}\varphi,\,Ae^{-isH}\varphi)|,\\&\quad\le 2\|\varphi\|\,\|A(H+I)^{-1}\|\,\|(H+I)\varphi\|\end{aligned}$$

which proves (51).

To conclude the proof we notice that (51) implies that $B(H+I)^{-1}$ is H-smooth. Since $\mathrm{Ran}(B^*)$ and $\mathrm{Ran}(H+I)^{-1}$ are dense, the closure of $\mathrm{Ran}(H+I)^{-1}B^*$ is $\mathscr{H}$. Theorem XIII.23 thus implies that $\mathscr{H}\subset\mathscr{H}_{ac}$. Therefore H has purely absolutely continuous spectrum. ∎

Corollary Let $m(N-1)\ge 3$. Let $\tilde H_0=\sum_{i=1}^{N}(-2\mu_i)^{-1}\Delta_i$ on $L^2(\mathbb{R}^{Nm})$ and let H_0 be $\tilde H_0$ with its center of mass motion removed. For each i, j suppose that $V_{ij}\colon\mathbb{R}^m\to\mathbb{R}$ and

(i) $V_{ij}\in L^p(\mathbb{R}^m)+L^\infty(\mathbb{R}^m)$ ($p=2$ if $m\le 3$, $p>2$ if $m=4$; $p=m/2$ if $m\ge 5$).

(ii) $\sum_{k=1}^{m}x_k\,\partial V_{ij}/\partial x_k\le 0$ in the distributional sense.

Then the operator $H=H_0+\sum_{i<j}V_{ij}(r_i-r_j)$ on $L^2(\mathbb{R}^{m(N-1)})$ has purely absolutely continuous spectrum.

Proof Let ζ be a Jacobi coordinate system so $H_0=\sum_{i=1}^{N-1}(-2M_i)^{-1}\Delta_{\zeta_i}$ and let $q_i=(2M_i)^{1/2}\zeta_i$ so $H_0=-\sum_{i=1}^{N-1}\Delta_{q_i}$. If we can show that $\sum_{i=1}^{N-1}q_i\cdot\nabla_{q_i}V_{jk}\le 0$ for all j,k, then the result follows from Theorem XIII.29. Suppose first that each V_{jk} is smooth. Then $V_{jk}=V_{jk}(\sum_{i=1}^{N-1}\alpha_iq_i)$ for suitable α_i. So

$$\sum_i q_i\cdot\nabla_{q_i}V_{jk}\Big(\sum_\ell\alpha_\ell q_\ell\Big)=\Big(\sum_i\alpha_iq_i\Big)\cdot(\nabla_rV_{jk})(r)\Big|_{r=\sum\alpha_\ell q_\ell}=(r\cdot\nabla_rV_{jk})(r)\Big|_{r=\sum\alpha_\ell q_\ell}$$

This is nonpositive by hypothesis. For arbitrary V_{jk}, we average with test functions and mimic the above argument. ∎

C. Local smoothness and wave operators for repulsive potentials

As a final topic in the theory of smooth operators, we shall discuss an extension of Theorem XIII.24. The "trouble" with that theorem is that its conclusion is too strong—H and H_0 are unitarily equivalent. In particular, the theorem cannot be applied to quantum Hamiltonians that have any pure point spectrum. We thus introduce a weaker notion than smoothness.

Definition Let H be a self-adjoint operator with spectral projections E_Ω. We say that A is ***H*-smooth on Ω**, a Borel set, if and only if AE_Ω is H-smooth.

Theorem XIII.30 Let H be self-adjoint with resolvent R and spectral projections $\{E_\Omega\}$. Let $\Omega\subset\mathbb{R}$. Suppose that $D(A)\supset D(H)$ and that *either*

(a) $\sup_{0<|\varepsilon|<1,\,\lambda\in\Omega}|\varepsilon|\,\|AR(\lambda+i\varepsilon)\|^2<\infty$

or

(b) $\sup_{0<\varepsilon<1,\,\lambda\in\Omega}\|AR(\lambda+i\varepsilon)A^*\|<\infty$

Then A is H-smooth on $\bar\Omega$, the closure of Ω.

Proof (a) For each $\varepsilon \neq 0$, $\|AR(\lambda + i\varepsilon)\|$ is continuous in λ, so the bound

$$C = \sup\{|\varepsilon| \|AR(\lambda + i\varepsilon)\|^2 \mid \lambda \in \Omega, 0 < |\varepsilon| < 1\}$$

extends to all $\lambda \in \bar{\Omega}$. Suppose $\lambda \in \mathbb{R}\backslash\bar{\Omega}$. Choose $\lambda_0 \in \bar{\Omega}$ with $|\lambda - \lambda_0| = \operatorname{dist}(\lambda, \bar{\Omega})$. Then

$$\begin{aligned}
&|\varepsilon| \|AR(\lambda + i\varepsilon)E_\Omega \varphi\|^2 \\
&\quad = |\varepsilon| \|AR(\lambda_0 + i\varepsilon)[I - (\lambda_0 - \lambda)R(\lambda + i\varepsilon)]E_{\bar{\Omega}}\varphi\|^2 \\
&\quad \leq |\varepsilon| \|AR(\lambda_0 + i\varepsilon)\|^2 \|(I - (\lambda_0 - \lambda)R(\lambda + i\varepsilon))E_{\bar{\Omega}}\|^2 \|\varphi\|^2 \\
&\quad \leq 4|\varepsilon| \|AR(\lambda_0 + i\varepsilon)\|^2 \|\varphi\|^2
\end{aligned}$$

since $|\lambda_0 - \lambda| \, |x - \lambda + i\varepsilon|^{-1} < 1$ for any $x \in \bar{\Omega}$. Thus

$$\sup_{\substack{\lambda \in \mathbb{R} \\ \varepsilon \neq 0}} |\varepsilon| \|AR(\lambda + i\varepsilon)E_{\bar{\Omega}}\| < \infty$$

so $AE_{\bar{\Omega}}$ is H-smooth by Theorem XIII.25 and the remark following its statement.

(b) Since $(AR(\lambda + i\varepsilon)A^*)^* = AR(\lambda - i\varepsilon)A^*$,

$$c = \sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} \|AR(\lambda + i\varepsilon)A^*\| < \infty$$

Thus

$$\begin{aligned}
&\sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} |\varepsilon| \|R(\lambda + i\varepsilon)A^*\|^2 \\
&\quad = \sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} |\varepsilon| \|AR(\lambda + i\varepsilon)R(\lambda - i\varepsilon)A^*\| \\
&\quad = \sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} \tfrac{1}{2}\|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]A^*\| \leq c < \infty
\end{aligned}$$

Since $\|R(\lambda + i\varepsilon)A^*\| = \|AR(\lambda - i\varepsilon)\|$, the conditions of (a) hold. ∎

We can now state the extension of Theorem XIII.24.

Theorem XIII.31 Let H and H_0 be self-adjoint operators with spectral projections E_Ω and $E_\Omega^{(0)}$. Suppose that

$$H - H_0 = A^*B$$

in the sense of (35). Suppose that A is H-bounded and H-smooth on some bounded open interval $\Omega \subset \mathbb{R}$ and that B is H_0-bounded and H_0-smooth on Ω. Then the limits

$$W_\pm = \operatorname*{s-lim}_{t \to \mp\infty} e^{iHt}e^{-iH_0t}E_\Omega^{(0)}$$

and

$$\tilde{W}_\pm = \operatorname*{s-lim}_{t \to \mp\infty} e^{iH_0t}e^{-iHt}E_\Omega$$

exist. Moreover,

$$W_\pm^* = \tilde{W}_\pm \tag{52}$$

$$\tilde{W}_\pm W_\pm = E_\Omega^{(0)}; \qquad W_\pm \tilde{W}_\pm = E_\Omega \tag{53}$$

Proof Suppose that we prove that $W_\pm$ exist and that Ran $W_\pm \subset E_\Omega$. Then, by symmetry, and the fact that $H_0 - H = -B^*A$, $\tilde{W}_\pm$ exist and Ran $\tilde{W}_\pm \subset E_\Omega^{(0)}$. (52) is obvious, and (53) follows from the fact that $W_\pm$ (respectively $W_\pm$) is a partial isometry with initial space $E_\Omega^{(0)}$ (respectively E_Ω). We shall show that $W_\pm$ exist and Ran $W_\pm \subset E_\Omega$ by proving that s-lim$_{t \to \mp\infty} E_\Omega e^{iHt}e^{-iH_0t}E_\Omega^{(0)}$ exists and

$$\operatorname*{s-lim}_{t \to \mp\infty} E_{\mathbb{R}\backslash\Omega}e^{iHt}e^{-iH_0t}E_\Omega^{(0)} = 0 \tag{54}$$

The proof that the first limit exists is identical to the proof of Theorem XIII.24. It is obviously sufficient to prove (54) with $E_\Omega^{(0)}$ replaced by $E_I^{(0)}$ for an arbitrary compact subinterval $I \subset \Omega$. Given such an I, let C be the contour in Figure XIII.4. Then

$$\begin{aligned}
&E_{\mathbb{R}\backslash\Omega}e^{iHt}e^{-iH_0t}E_I^{(0)}\varphi \\
&\quad = \frac{1}{2\pi i}\oint_C E_{\mathbb{R}\backslash\Omega}(H - z)^{-1}e^{iHt}e^{-iH_0t}E_I^{(0)}\varphi \, dz \\
&\qquad - \frac{1}{2\pi i}\oint_C E_{\mathbb{R}\backslash\Omega}e^{iHt}e^{-iH_0t}(H_0 - z)^{-1}E_I^{(0)}\varphi \, dz \\
&\quad = \frac{1}{2\pi i}\oint_C E_{\mathbb{R}\backslash\Omega}e^{iHt}[(H - z)^{-1} - (H_0 - z)^{-1}]e^{-iH_0t}E_I^{(0)}\varphi \, dz
\end{aligned}$$

Since this last integrand is uniformly bounded on C, it is sufficient, by the dominated convergence theorem, to prove that

$$\operatorname*{s-lim}_{t \to \mp\infty}[(H - z)^{-1} - (H_0 - z)^{-1}]e^{-iH_0t}E_I^{(0)} = 0 \tag{55}$$

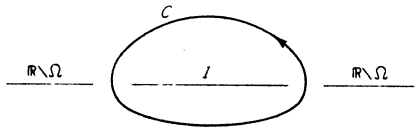


FIGURE XIII.4 A contour of integration.

for all nonreal z. But

$$\begin{aligned}|(\psi, [(H-z)^{-1} - (H_0-z)^{-1}]e^{-iH_0t}E_I^{(0)}\varphi)| \\ = |(A(H-z)^{-1}\psi, B(H_0-z)^{-1}e^{-iH_0t}E_I^{(0)}\varphi)| \\ \leq \|A(H-z)^{-1}\| \, \|B(H_0-z)^{-1}e^{-iH_0t}E_I^{(0)}\varphi\| \, \|\psi\|\end{aligned}$$

Thus, to prove (55) we need only show

$$\lim_{t\to\pm\infty} \|B(H_0-z)^{-1}e^{-iH_0t}E_I^{(0)}\varphi\| = 0 \tag{56}$$

But, by the smoothness hypothesis, the function of t in (56) is square-integrable. Moreover, it has a uniformly bounded derivative, so (56) holds (Problem 62). ∎

Corollary Suppose that H and H_0 are self-adjoint with spectral projections E_Ω and $E_\Omega^{(0)}$ and that

$$H - H_0 = A^*B$$

where B is H_0-bounded and A is H-bounded. Let $S \subset \mathbb{R}$ with $S = \bigcup_{i=1}^\infty \Omega_i$ and each Ω_i a bounded open interval. Suppose that:

(i) A is H-smooth on each Ω_i and B is H_0-smooth on each Ω_i.
(ii) Both $\sigma(H)\backslash S$ and $\sigma(H_0)\backslash S$ have Lebesgue measure zero.

Then the generalized wave operators $\text{s-lim}_{t\to\mp\infty} e^{iHt}e^{-iH_0t}E_{\text{ac}}^{(0)}$ exist and are complete.

Proof Since $S = \bigcup_{i=1}^\infty \Omega_i$ and $E_{\text{ac}}^{(0)} = E_S^{(0)}$, existence follows if we can prove that $\lim_{t\to\mp\infty} e^{iHt}e^{-iH_0t}\varphi$ exists for $\varphi \in \bigcup_{i=1}^\infty \text{Ran}\, E_{\Omega_i}^{(0)}$. This is a direct consequence of the theorem. Since the inverse wave operators exist by symmetry, the wave operators are complete. ∎

One application of this corollary will be given in Section 8. Here we apply it to prove a result in the theory of repulsive potentials. This result is not the best possible (see the Notes).

Theorem XIII.32 Let H be an operator of the form given in the corollary of Theorem XIII.29. Suppose that each V_{ij} is a function of $|x|$ obeying $|V_{ij}(x)| \leq C(1+|x|)^{-\frac{1}{2}-\varepsilon}$ for each i and j and some $\varepsilon > 0$. Then the wave operators $\Omega^\pm = \text{s-lim}_{t\to\mp\infty} e^{iHt}e^{-iH_0t}$ exist and are unitary.

Proof Since we already know that H has purely absolutely continuous spectrum, it is sufficient to prove that the wave operators exist and are complete. In the notation used in the proof of Theorem XIII.29, let

$$A_{jk} = +i\left|g(r_j - r_k)\frac{d}{dr_{jk}} + \frac{d}{dr_{jk}}g(r_j - r_k)\right|, \qquad A = \sum_{j=k} A_{jk}$$

where $r_{jk} = |r_j - r_k|$ and d/dr_{jk} is defined by

$$r_{jk}\frac{d}{dr_{jk}} = (r_j - r_k)\cdot(\nabla_j - \nabla_k)$$

Now, $i[A_{ij}, V_{ij}] \geq 0$ as in the proof of Theorem XIII.29 and $i[A_{k\ell}, V_{ij}] = 0$ for i, j, k, ℓ distinct. Finally, for i, j, k distinct,

$$i[A_{ik} + A_{kj}, V_{ij}(r_{ij})] = \mathbf{a}(i,j,k)\cdot(\nabla V_{ij})(r_{ij})$$

where $\mathbf{a}(i,j,k) = g(r_{ik})\mathbf{e}_{ik} + g(r_{kj})\mathbf{e}_{kj}$ and $\mathbf{e}_{ik} = r_{ik}^{-1}(\mathbf{r}_i - \mathbf{r}_k)$. Since V_{ij} is only a function of $|x|$ and $(\mathbf{x}\cdot\nabla)V_{ij} \leq 0$, we can conclude that $i[A_{ik} + A_{kj}, V_{ij}] \geq 0$ if $(\mathbf{r}_i - \mathbf{r}_j)\cdot(\mathbf{a}(i,j,k)) \geq 0$. But

$$\begin{aligned}(\mathbf{r}_i - \mathbf{r}_j)\cdot\mathbf{a}(i,j,k) &= r_{ik}g(r_{ik}) + r_{kj}g(r_{kj}) \\ &\quad + (e_{ik}\cdot e_{kj})(r_{ik}g(r_{kj}) + r_{kj}g(r_{ik})) \\ &\geq (r_{ik} - r_{kj})(g(r_{ik}) - g(r_{jk})) \\ &\geq 0\end{aligned}$$

since g is monotone. It follows that $i[A, V] \geq 0$ so that computations identical to those used in Theorem XIII.29 show that (Problem 64):

$$i[A, H] \geq c(1 + r_{jk})^{-3-\varepsilon}$$

for a suitable constant c. Again, following the proof of Theorem XIII.29, we conclude that $(1+r_{jk})^{-\frac{1}{2}-\varepsilon}(H+I)^{-1}$ is H-smooth. Since

$$\| \, |V_{ij}|^{3/5}(H+I)^{-1}e^{-iHt}\varphi\| \leq c^{1/2}\|(1+r_{jk})^{-\frac{1}{2}-\varepsilon}(H+I)^{-1}e^{-iHt}\varphi\|$$

$|V_{ij}|^{3/5}(H+I)^{-1}$ is H-smooth and thus $|V_{ij}|^{3/5}$ is H-smooth on any compact set. By hypothesis, $|V_{ij}|^{2/5} \in L^{m+\varepsilon}(\mathbb{R}^m) \cap L^{m-\varepsilon}(\mathbb{R}^m)$, so by the proof of Theorem XIII.27, $|V_{ij}|^{2/5}$ is H_0-smooth. The result now follows from the previous corollary. ∎

XIII.8 The absence of singular continuous spectrum III: Weighted L^2 spaces

We have seen that a sufficient condition for $\sigma_{\text{sing}}(H)$ to be empty is that there be a dense set of vectors $X \subset \mathscr{H}$ so that $(\varphi, (H - z)^{-1}\varphi)$ remains bounded as $z \to \lambda \in \mathbb{R}$ for any $\varphi \in X$. There is a natural way of approaching this condition. Suppose that $X \subset \mathscr{H}$ is dense and that there is a norm $|||\cdot|||_+$ on X so that X is a Banach space and so that $|||\varphi|||_+ \geq \|\varphi\|$ for any $\varphi \in X$. Then the inner product on $\mathscr{H}$ allows one to realize $\mathscr{H}$ in a natural way as a subset of X^*. If $|||\cdot|||_-$ denotes the norm on X^*, then $\|\varphi\| \geq |||\varphi|||_-$ for any $\varphi \in \mathscr{H}$. We have already discussed such a situation and related ideas in Section VIII.6 and the appendix to Section XI.6. Let $z \in \mathbb{C}$ with $\operatorname{Im} z \neq 0$. Then $(H - z)^{-1}$ takes $\mathscr{H}$ into $\mathscr{H}$ and so X into X^*. Of course the norm of $(H - z)^{-1}$ as a map from $\mathscr{H}$ to $\mathscr{H}$ diverges as z approaches $\sigma(H)$, but suppose that it remains bounded as a map of X into X^*. Then

$$|(\varphi, (H - z)^{-1}\varphi)| \leq |||\varphi|||_+^2 \, \|(H - z)^{-1}\|_{+,-}$$

where

$$\|A\|_{+,-} = \sup_{\psi \neq 0, \psi \in X} \|A\psi\|_- / \|\psi\|_+$$

so we can conclude that $\sigma_{\text{sing}}(H) = \varnothing$, by Theorem XIII.20.

It is natural to try to implement this idea with perturbation techniques. That is, we consider $H = H_0 + V$ and begin by proving bounds on $(H_0 - z)^{-1}$ as a map from X to X^*. We shall consider Schrödinger operators and take $H_0 = -\Delta$. To motivate our choice of X, let $f \in \mathscr{S}(\mathbb{R}^n)$ and consider

$$\begin{aligned} &\lim_{y \downarrow 0} (f, [(H_0 - x + iy)^{-1} - (H_0 - x - iy)^{-1}]f) \\ &\quad = \lim_{y \downarrow 0} \int |\hat{f}(p)|^2 2i \operatorname{Im}[(p^2 - x + iy)^{-1}] \, d^n p \\ &\quad = -2i\pi \int |\hat{f}(p)|^2 \, \delta(p^2 - x) \, d^n p \end{aligned}$$

by Eq. (V.4). Thus, for $(f, (H_0 - x + iy)^{-1}f)$ to have a limit as $y \downarrow 0$, $\hat{f}$ must have a "natural" restriction to the sphere of radius $x^{1/2}$. Because of our discussion in Section IX.9, it is natural to choose X as an L^2_δ space (with $\delta > \frac{1}{2}$) so that X^* is $L^2_{-\delta}$:

$$L^2_\delta(\mathbb{R}^n) = \left\{ f(x) \,\middle|\, \|f\|_\delta^2 \equiv \int (1 + x^2)^\delta |f(x)|^2 \, dx < \infty \right\}$$

We shall lean heavily on the estimates proven in Section IX.9, especially Theorems IX.39 and IX.41.

Definition A multiplication operator is called an **Agmon potential** if $V(x) = (1 + x^2)^{-\frac{1}{2}-\varepsilon}W(x)$ for some $\varepsilon > 0$ and some W that is a relatively compact perturbation of $-\Delta$.

The Agmon potentials form a vector space of $-\Delta$-bounded perturbations of relative bound zero (see Problem 20 of Chapter X).

Example 1 Let $p > n/2$, $p < \infty$, and $p \geq 2$. Then any $W \in L^p(\mathbb{R}^n)$ is relatively compact (Problem 41), so any V with $(1 + x^2)^{\frac{1}{2}+\varepsilon}V \in L^p$ is an Agmon potential.

Example 2 Let $W \in L^\infty(\mathbb{R}^n)$ and define $V(x) = (1 + x^2)^{-\frac{1}{2}-\varepsilon}W(x)$. To show that V is an Agmon potential we need only prove that $U(x) = (1 + x^2)^{-\varepsilon/2}W(x)$ is relatively compact. But this is true since $U(x)$ is in $L^p + (L^\infty)_\varepsilon$ for all p (Problem 41).

The main theorem of this section is:

Theorem XIII.33 (the Agmon–Kato–Kuroda theorem) Let V be an Agmon potential and let $H = H_0 + V$ where $H_0 = -\Delta$. Then:

(a) The set $\mathscr{E}_+$ of positive eigenvalues of H is a discrete subset of $(0, \infty)$, and each eigenvalue has finite multiplicity.
(b) If C is any compact subinterval of $(0, \infty)\backslash\mathscr{E}_+$ and if $\delta > \frac{1}{2}$, then

$$\sup_{\lambda \in C, 0 < y < 1} \sup_{\psi, \varphi \in L^2_\delta: \|\varphi\|_\delta \leq 1, \|\psi\|_\delta \leq 1} |(\psi, (H - \lambda - iy)^{-1}\varphi)| < \infty$$

(c) $\sigma_{\text{sing}}(H) = \varnothing$.
(d) The wave operators $\Omega^\pm(H, H_0)$ exist and are complete.

The proof of Theorem XIII.33, while elegant, is rather long so we break it up into a series of lemmas. After proving (a), we develop a few technical estimates that will allow us to prove (c) and (d) from (b); then we prove (b) in case $V = 0$; finally, we use the estimates proven for H_0, Theorem IX.39, Theorem IX.41, and a bootstrap argument to complete the proof. Throughout we let $\rho(x) \equiv (1 + x^2)^{1/2}$. The use of the weighted L^2 spaces and Theorem IX.39 is illustrated in:

Proof of (a) of Theorem XIII.33 Suppose that $\varphi \in D(H)$ and $H\varphi = \lambda\varphi$ with $\lambda > 0$. First, we shall show that $\|\varphi\|_\delta \leq c\|\varphi\|$ for some $\delta > 0$ where c depends only on λ and remains bounded as λ varies through compact subsets of

$(0, \infty)$. Since W is H_0-compact, it is H-bounded so that $\|W\varphi\| \leq a\|H\varphi\| + b\|\varphi\| = (a\lambda + b)\|\varphi\|$. As a result $\psi \equiv V\varphi = \rho^{-1-\varepsilon}W\varphi$ is in $L^2_{1+\varepsilon}$. In particular, by Theorem IX.40, $\hat{\psi}$ has restrictions to each sphere S_E, and the restriction is Hölder continuous in E. Since $(H_0 - \lambda)\varphi = -\psi$, $\hat{\varphi} = -(k^2 - \lambda)^{-1}\hat{\psi}$. If $\hat{\psi} \restriction S_{\sqrt{\lambda}}$ were not identically zero, then $\hat{\varphi}$ could not be in L^2, so we conclude that $\psi \restriction S_{\sqrt{\lambda}} = 0$. As a result, Theorem IX.41 is applicable, so

$$\|\varphi\|_{\varepsilon/2} \leq c_\lambda \|\psi\|_{1+\varepsilon} = c_\lambda \|W\varphi\| \leq d_\lambda \|\varphi\|$$

Let $\eta \equiv \rho^{\varepsilon/2}(-\Delta + 1)\varphi$. Then $H\varphi = \lambda\varphi$ implies that

$$\begin{aligned}\|\eta\| &\leq \|\rho^{\varepsilon/2}(\lambda + 1)\varphi\| + \|\rho^{\varepsilon/2}V\varphi\| \\ &\leq (\lambda + 1)\|\varphi\|_{\varepsilon/2} + \|W\varphi\| \leq c'_\lambda \|\varphi\|\end{aligned}$$

Since $\varphi = (-\Delta + 1)^{-1}\rho^{-\varepsilon}\eta$, we conclude that for any compact subset K in $(0, \infty)$, any solution of $H\varphi = \lambda\varphi$ with $\lambda \in K$ and $\|\varphi\| = 1$ is of the form $\varphi = A\eta$ where: (i) $A = (-\Delta + 1)^{-1}\rho^{-\varepsilon}$ and (ii) $\|\eta\| \leq c$, a constant only depending on K. By Problem 41, A is a compact operator, so the set $M = \{\varphi = A\eta \mid \|\eta\| \leq c\}$ is compact. If any eigenvalue $\lambda \in K$ were of infinite multiplicity or if there were infinitely many eigenvalues in K, M would contain an infinite orthonormal set. Since M is compact, K contains only finitely many eigenvalues and each is of finite multiplicity. ∎

We note that we shall show that $\mathscr{E}_+ = \varnothing$ under some additional regularity hypotheses on V in Section 13.

Lemma 1 Let F and G be any two real-valued multiplication operators that are H_0-bounded with relative bound zero. Then for any $\mu \in \mathbb{C}\backslash\mathbb{R}$, $(H_0 - \mu)^{-1}$, $(H_0 + G - \mu)^{-1}$, $F(H_0 - \mu)^{-1}$, and $F(H_0 + G - \mu)^{-1}$ are bounded on each L^2_δ. Moreover, if F is also H_0-relatively compact, then $F(H_0 - \mu)^{-1}$ and $F(H_0 + G - \mu)^{-1}$ are compact on each L^2_δ.

Proof We shall prove the lemma for $(H_0 - \mu)^{-1}$ in the case $|\delta| \leq 1$. The other cases are similar and are left to the problems (Problem 66). Introduce the symbol ∂_j for the operator $\partial/\partial x_j$ and consider the formal computation

$$\begin{aligned}[(H_0 - \mu)^{-1}, \rho^\delta] &= -(H_0 - \mu)^{-1}[H_0, \rho^\delta](H_0 - \mu)^{-1} \\ &= \sum_{i=1}^{n} \{(H_0 - \mu)^{-1}\partial_i\}(\partial_i\rho^\delta)(H_0 - \mu)^{-1} \\ &\quad + (H_0 - \mu)^{-1}(\partial_i\rho^\delta)\{\partial_i(H_0 - \mu)^{-1}\}\end{aligned}$$

Applied to vectors in $\mathscr{S}$, all computations are legitimate. Moreover, if $\delta \leq 1$, $\partial_i(\rho^\delta)$ is bounded. Since $(H_0 - \mu)^{-1}$ and $\partial_i(H_0 - \mu)^{-1}$ are bounded on L^2 we conclude that

$$\|[(H_0 - \mu)^{-1}, \rho^\delta]\psi\| \leq \text{const}\|\psi\|$$

if ψ is in $\mathscr{S}$ and so for arbitrary ψ in L^2. Suppose $1 \geq \delta > 0$. Then

$$\begin{aligned}\|(H_0 - \mu)^{-1}\psi\|_\delta &= \|\rho^\delta(H_0 - \mu)^{-1}\psi\| \\ &\leq \|(H_0 - \mu)^{-1}\| \, \|\psi\|_\delta + \|[(H_0 - \mu)^{-1}, \rho^\delta]\psi\| \\ &\leq d\|\psi\|_\delta\end{aligned}$$

so $(H_0 - \mu)^{-1}$ is bounded from L^2_δ to L^2_δ. By duality, $(H_0 - \bar{\mu})^{-1}$ is bounded from $L^2_{-\delta}$ to $L^2_{-\delta}$. ∎

Lemma 2 Let $H = H_0 + V$ as in Theorem XIII.33. Suppose that F is an Agmon potential and that for some compact interval $\Omega \subset \mathbb{R}$, and each $\delta > \frac{1}{2}$,

$$\sup_{x \in \Omega,\, 0 < y < 1} \; \sup_{\psi, \varphi \in L^2_\delta;\, \|\varphi\|_\delta \leq 1,\, \|\psi\|_\delta \leq 1} |(\psi, (H - \lambda - iy)^{-1}\varphi)| < \infty \quad (57)$$

Then $|F|^{1/2}$ is H-smooth on Ω.

Proof By Theorem XIII.30, we need only prove that

$$\sup_{\substack{\lambda \in \Omega \\ 0 < y < 1}} \| \, |F|^{1/2}(H - \lambda - iy)^{-1}|F|^{1/2}\| < \infty$$

(57) implies that $(H - \lambda - iy)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ for $\lambda + iy \in \Omega \times (0, 1)$. Write $F = \rho^{-1-\varepsilon}G$ where G is H_0-compact and let $\delta = \frac{1}{2} + (\varepsilon/2)$. Then, by Lemma 1, $(H - i)^{-1}|G|^{1/2}$ is bounded from L^2_δ to L^2_δ so $|G|^{1/2}(H - i)^{-1}(H - \lambda - iy)^{-1}(H - i)^{-1}|G|^{1/2}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ for $\lambda + iy \in \Omega \times (0, 1)$. Thus

$$|F|^{1/2}(H - i)^{-1}(H - \lambda - iy)^{-1}(H - i)^{-1}|F|^{1/2}$$

is uniformly bounded from L^2 to L^2 for $\lambda + iy \in \Omega \times (0, 1)$. Writing

$$\begin{aligned}(H - z)^{-1} &= (H - i)^{-1} + (z - i)(H - i)^{-2} \\ &\quad + (z - i)^2(H - i)^{-1}(H - z)^{-1}(H - i)^{-1}\end{aligned}$$

and using the fact that $\| \, |F|^{1/2}(H - i)^{-1}|F|^{1/2}\| < \infty$, we see that

$$\sup_{\lambda + iy \in \Omega \times (0,1)} \| \, |F|^{1/2}(H - \lambda - iy)^{-1}|F|^{1/2}\| < \infty. \; ∎$$

Reduction of Theorem XIII.33 to the proof of (b) We want to show that once we prove (b), then (c) and (d) follow. Suppose that (b) holds, that $\varphi \in L^2_\delta$ for $\delta > \frac{1}{2}$, and that K is a compact subinterval of $(0, \infty)\backslash\mathscr{E}_+$. Then $E_K\varphi \in \mathscr{H}_{ac}$ by Theorem XIII.20. Thus $K \cap \sigma_{sing} = \varnothing$. By the second corollary to Theorem XIII.14, $\sigma_{ess} = [0, \infty)$, so we conclude that $\sigma_{sing} \cap (-\infty, 0) = \varnothing$. Therefore, $\sigma_{sing} \subset (\mathscr{E}_+ \cup \{0\})$. $\mathscr{E}_+$ is countable by (a), so $\sigma_{sing} = \varnothing$. Applying Lemma 2 to the case $V = 0$, we see that $|V|^{1/2}$ is H_0-smooth on Ω for any interval $[a, b]$ with $a > 0$. In addition, $|V|^{1/2}$ is H-smooth on any such Ω with $\Omega \cap \mathscr{E}_+ = \varnothing$. (d) now follows from the corollary of Theorem XIII.31. ∎

The remainder of this section is devoted to proving (b). We first prove the case $V = 0$, which is an estimate quite similar to Theorem IX.41. The proof is also quite similar.

Lemma 3 Let $\varepsilon > 0$. Then there exists a constant c so that for all $\lambda \in \mathbb{C}$ and all $\varphi \in \mathscr{S}(\mathbb{R})$

$$\|\varphi\|_{-\frac{1}{2}-\varepsilon} \leq c\left\|\left(\frac{d}{dx} - \lambda\right)\varphi\right\|_{\frac{1}{2}+\varepsilon} \tag{58}$$

Proof Suppose that $\operatorname{Re}\lambda \leq 0$. Let $\psi = (d/dx - \lambda)\varphi$. Then

$$\varphi(x) = \int_{-\infty}^{x} e^{\lambda(x-y)}\psi(y)\,dy$$

Thus

$$\begin{aligned}\|\varphi\|_{L^\infty} &\leq \|\psi\|_{L^1} = ((1+x^2)^{-\frac{1}{2}-\frac{1}{2}\varepsilon}, (1+x^2)^{\frac{1}{2}+\frac{1}{2}\varepsilon}\psi) \\ &\leq c_1\|\psi\|_{\frac{1}{2}+\varepsilon}\end{aligned}$$

Since

$$\|\varphi\|_{-\frac{1}{2}-\varepsilon} \leq \|\varphi\|_{L^\infty}\|(1+x^2)^{-\frac{1}{2}-\frac{1}{2}\varepsilon}\|_{L^2}$$

(58) follows in the case $\operatorname{Re}\lambda \leq 0$. A similar argument works for $\operatorname{Re}\lambda \geq 0$. ∎

Lemma 4 Let n be fixed. Then for all $\varepsilon > 0$, there is a constant d so that for all $\lambda \in \mathbb{C}$, each $j = 1, \ldots, n$, and all $\varphi \in \mathscr{S}(\mathbb{R}^n)$,

$$\|\partial_j\varphi\|_{-\frac{1}{2}-\varepsilon} \leq d\|(-\Delta - \lambda)\varphi\|_{\frac{1}{2}+\varepsilon} \tag{59}$$

Proof Consider first the case $n = 1$. Let $\lambda = -\mu^2$. Then by Lemma 3,

$$\begin{aligned}\left\|\frac{d}{dx}\varphi\right\|_{-\frac{1}{2}-\varepsilon} &\leq \frac{1}{2}\left\|\left(\frac{d}{dx} - \mu\right)\varphi\right\|_{-\frac{1}{2}-\varepsilon} + \frac{1}{2}\left\|\left(\frac{d}{dx} + \mu\right)\varphi\right\|_{-\frac{1}{2}-\varepsilon} \\ &\leq c\left\|\left(-\frac{d^2}{dx^2} - \lambda\right)\varphi\right\|_{\frac{1}{2}+\varepsilon}\end{aligned}$$

Now let $\varphi \in \mathscr{S}(\mathbb{R}^n)$ and let $\psi(x_1, k_2, \ldots, k_n)$ be the partial Fourier transform of φ with respect to $x_2, \ldots, x_n$,

$$\psi(x_1, k_2, \ldots, k_n) = (2\pi)^{-(n-1)/2}\int e^{-i\sum_2^n k_j x_j}\varphi(x_1, \ldots, x_n)\,dx_2 \cdots dx_n$$

Using the one-dimensional result, for each fixed $k_2, \ldots, k_n$,

$$\begin{aligned}&\int (1+x_1^2)^{-\frac{1}{2}-\varepsilon}|\partial_1\psi(x_1, k_2, \ldots, k_n)|^2\,dx_1 \\ &\quad\leq c\int (1+x_1^2)^{\frac{1}{2}+\varepsilon}|(-\partial_1^2 + k_2^2 + \cdots + k_n^2 - \lambda)\psi|^2\,dx_1\end{aligned}$$

Integrating with respect to $k_2, \ldots, k_n$ and using the Plancherel theorem, we see that

$$\int (1+x_1^2)^{-\frac{1}{2}-\varepsilon}|\partial_1\varphi(x)|^2\,d^nx \leq c\int (1+x_1^2)^{\frac{1}{2}+\varepsilon}|(-\Delta - \lambda)\varphi|^2\,d^nx$$

Since $(1+x^2)^{-\frac{1}{2}-\varepsilon} \leq (1+x_1^2)^{-\frac{1}{2}-\varepsilon}$ and $(1+x_1^2)^{\frac{1}{2}+\varepsilon} \leq (1+x^2)^{\frac{1}{2}+\varepsilon}$, (59) follows. ∎

Lemma 5 Let n be fixed. For any compact set $K \subset \mathbb{C}\backslash\{0\}$, there is a constant c so that for all $\lambda \in K$ and $\varphi \in \mathscr{S}(\mathbb{R}^n)$,

$$\|\varphi\|_{-\frac{1}{2}-\varepsilon} \leq c\|(-\Delta - \lambda)\varphi\|_{\frac{1}{2}+\varepsilon} \tag{60}$$

Proof We can find $c_1 > 0$ satisfying

$$\inf_{x\in\mathbb{R},\,\lambda\in K}[|x^2 - \lambda|^2 + |x|^2] \geq c_1^{-2}$$

Therefore, given $\psi \in \mathscr{S}(\mathbb{R}^n)$

$$|\hat{\psi}(k_1, \ldots, k_n)|^2 \leq c_1^2\left|\,|(\textstyle\sum k_i^2 - \lambda)\hat{\psi}(k_1, \ldots, k_n)|^2 + \sum_{i=1}^n |k_i\hat{\psi}(k_1, \ldots, k_n)|^2\right|$$

Integrating and using the Plancherel theorem

$$\|\psi\|^2 \leq c_1^2\left|\,\|(-\Delta - \lambda)\psi\|^2 + \sum_{j=1}^n \|\partial_j\psi\|^2\right| \tag{61a}$$

for all $\lambda \in K$. Let α be a positive real number which we shall adjust below. Set $\delta = \frac{1}{2} + \varepsilon$ and $\rho_\alpha = (1 + \alpha x^2)^{1/2}$. Finally, let $\varphi = (\rho_\alpha)^\delta \psi$. Then, by (61a)

$$\|\rho_\alpha^{-\delta}\varphi\| \leq c_1 \|(-\Delta - \lambda)\rho_\alpha^{-\delta}\varphi\| + c_1 \sum_{j=1}^{n} \|\partial_j \rho_\alpha^{-\delta}\varphi\| \tag{61b}$$

Now $\partial_j \rho_\alpha^{-\delta}\varphi = \rho_\alpha^{-\delta}\,\partial_j\psi - \delta\alpha x_j \rho_\alpha^{-\delta-1}\varphi$ so

$$\|\partial_j \rho_\alpha^{-\delta}\varphi\| \leq \|\rho_\alpha^{-\delta}\,\partial_j\varphi\| + \alpha^{1/2}\,\delta\|\rho_\alpha^{-\delta}\varphi\|$$

since $|\alpha^{1/2} x_j \rho^{-1}| \leq 1$ for all x. Similarly (Problem 67),

$$\|(-\Delta - \lambda)\rho_\alpha^{-\delta}\varphi\| \leq \|\rho_\alpha^{-\delta}(-\Delta - \lambda)\varphi\| + 2\,\delta\alpha^{1/2} \sum_{j=1}^{n} \|\rho_\alpha^{-\delta}\,\partial_j\varphi\| + d_{n,\varepsilon}\alpha\|\rho_\alpha^{-\delta}\varphi\| \tag{62}$$

where $d_{n,\varepsilon}$ is only dependent on ε and n. Pick α so small that $c_1(n\,\delta\alpha^{1/2} + d_{n,\varepsilon}\alpha) < \frac{1}{2}$ and $\alpha < 1$. Then, by (61), for all $\varphi \in \mathscr{S}$ and $\lambda \in K$,

$$\tfrac{1}{2}\|\rho_\alpha^{-\delta}\varphi\| \leq c_2 \left\| \|\rho_\alpha^{-\delta}(-\Delta - \lambda)\varphi\| + \sum_{j=1}^{n} \|\rho_\alpha^{-\delta}\,\partial_j\varphi\| \right|$$

Since $\rho^{-\delta} \leq \rho_\alpha^{-\delta} \leq \alpha^{-\delta/2}\rho^{-\delta}$, we have that

$$\|\varphi\|_{-\delta} \leq c_3[\|(-\Delta - \lambda)\varphi\|_{-\delta} + \sum_j \|\partial_j\varphi\|_{-\delta}]$$

where c_3 is independent of $\lambda \in K$ and $\varphi \in \mathscr{S}$. Since $\|\cdot\|_{-\delta} \leq \|\cdot\|_\delta$ and $\|\partial_j\varphi\|_{-\delta} \leq c\|(-\Delta - \lambda)\varphi\|_\delta$ by Lemma 4, (60) follows. ∎

If now $\operatorname{Im}\lambda \neq 0$ and $\delta > \frac{1}{2}$, then by Lemma 1, $(H_0 - \lambda)^{-1}$ is a bounded map from L^2_δ to $L^2_{-\delta}$. Lemma 5 assures us that, for $\lambda \in K = [a, b] \times (0, 1]$ ($a > 0$), we have the basic estimate

$$\|(H_0 - \lambda)^{-1}\varphi\|_{-\delta} \leq c\|\varphi\|_\delta \tag{63}$$

Given (63), it is natural to consider the boundary values $\lim_{y \downarrow 0} (H_0 - x - iy)^{-1}$ as maps of L^2_δ to $L^2_{-\delta}$. Such boundary values are not strictly necessary for the proof, but they help to make it more conceptual, so we introduce them. As preparation, we need

Lemma 6 Let $\delta > \frac{1}{2}$ and let $0 < a < b$. Then there is a constant c so that for all $\varphi \in L^2_\delta$ and $\lambda = x + iy$ with $x \in [a, b]$ and $y \in (0, 1]$,

$$\|(H_0 - \lambda)^{-2}\varphi\|_{-\delta} \leq c\|\varphi\|_\delta$$

Proof Let A be the operator $\sum_{j=1}^n x_j \partial_j$. Then $[A, (H_0 - \lambda)] = -2H_0$ so that

$$\begin{aligned}[A, (H_0 - \lambda)^{-1}] &= -(H_0 - \lambda)^{-1}[A, (H_0 - \lambda)](H_0 - \lambda)^{-1} \\ &= 2H_0(H_0 - \lambda)^{-2} \\ &= 2(H_0 - \lambda)^{-1} + 2\lambda(H_0 - \lambda)^{-2}\end{aligned}$$

where all the computations are legitimate when applied to vectors in $\mathscr{S}(\mathbb{R}^n)$. Since $(H_0 - \lambda)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$, we need only prove that $[A, (H_0 - \lambda)^{-1}]$ is bounded from L^2_δ to $L^2_{-\delta}$, uniformly for λ satisfying $a \leq \operatorname{Re}\lambda \leq b$, $0 < \operatorname{Im}\lambda \leq 1$. It is thus sufficient to prove that $\rho^{-\delta}(x_j\partial_j) \times (H_0 - \lambda)^{-1}\rho^{-\delta}$ is bounded on L^2 uniformly in λ. Write

$$(H_0 - \lambda)^{-1} = (H_0 + 1)^{-1} + (\lambda + 1)(H_0 + 1)^{-1}(H_0 - \lambda)^{-1}$$

Certainly $(\rho^{-\delta}x_j)[\partial_j(H_0 + 1)^{-1}]\rho^{-\delta}$ is bounded on L^2. Moreover

$$\rho^{-1}x_j[\rho^{-\delta+1}(\partial_j(H_0 + 1)^{-1})\rho^{\delta-1}](\rho^{-\delta+1}(H_0 - \lambda)^{-1}\rho^{-\delta+1})\rho^{-1}$$

is bounded for the first and last factor are trivially bounded, the third is bounded by Lemma 5, and the second is bounded by mimicking the proof of Lemma 1 (Problem 66c). ∎

Lemma 7 Let $\delta > \frac{1}{2}$ and let $x > 0$. Then $(H_0 - x - i0)^{-1} \equiv \lim_{y \downarrow 0} (H_0 - x - iy)^{-1}$ exists in norm as a map from L^2_δ to $L^2_{-\delta}$. Moreover:

(a) $V(H_0 - x - i0)^{-1}$ is compact as a map of L^2_δ to L^2_δ if V is an Agmon potential such that $\rho^{2\delta}V = W$ is relatively H_0-compact.

(b) $\operatorname{Im}(\varphi, (H_0 - x - i0)^{-1}\varphi) = (\pi/2)x^{\frac{1}{2}n-1} \int_{S^{n-1}} |\hat{\varphi}(x^{1/2}\Omega)|^2\, d\Omega$ where $\hat{\varphi} \restriction S_{x^{1/2}}$ is defined by Theorem IX.39, and $d\Omega$ is the usual surface measure on the sphere.

Proof Let $\delta' = \delta + 1$. Then as operators from $L^2_{\delta'}$ to $L^2_{-\delta'}$

$$\begin{aligned}&\|(H_0 - \lambda_1)^{-1} - (H_0 - \lambda_2)^{-1}\| \\ &\quad \leq |\lambda_2 - \lambda_1| \sup_{0 \leq t \leq 1} \|[H_0 - t\lambda_1 - (1 - t)\lambda_2]^{-2}\|\end{aligned}$$

By Lemma 6, we see that $(H_0 - x - iy)^{-1}$ is norm Cauchy as $y \downarrow 0$. Let $\delta'' = \frac{1}{2}(\delta + \frac{1}{2})$. Then by Lemma 5, $(H_0 - x - iy)^{-1}$ is norm bounded as $y \downarrow 0$ as a map from $L^2_{\delta''}$ to $L^2_{-\delta''}$. Since $\delta'' < \delta < \delta'$, we can interpolate between the

δ' and δ'' results (see Example 3 of the appendix to Section IX.4) and conclude that as maps from L^2_δ to $L^2_{-\delta}$, $(H_0 - x - iy)^{-1}$ is norm Cauchy as $y \downarrow 0$. To prove (a) we write

$$W(H_0 - x - i0)^{-1} = W(H_0 + 1)^{-1} + (x + 1)W(H_0 + 1)^{-1}(H_0 - x - i0)^{-1}$$

and so conclude by Lemma 1 that $W(H_0 - x - i0)^{-1}$ is compact as a map from L^2_δ to $L^2_{-\delta}$. Since $\rho^{-2\delta}$ is an isometry from $L^2_{-\delta}$ to L^2_δ, (a) follows. Finally, (b) holds for $\varphi \in \mathscr{S}$ because of (V.4) (see Problem 22 of Chapter V). By Theorem IX.39, it extends to all $\varphi \in L^2_\delta$. ∎

Lemma 8 Let $\delta > \frac{1}{2}$ and let $\varphi \in L^2_\delta$ satisfy $\varphi = -V(H_0 - x - i0)^{-1}\varphi$ where $x > 0$, and V is an Agmon potential so that $\rho^{2\delta}V = W$ is relatively H_0-compact, and where $V(H_0 - x - i0)^{-1}$ is interpreted as the composition of maps $W(H_0 - x - i0)^{-1}$ from L^2_δ to $L^2_{-\delta}$ and $\rho^{-2\delta}$ from $L^2_{-\delta}$ to L^2_δ. Then:

(a) $\psi \equiv (H_0 - x - i0)^{-1}\varphi$ is in L^2.
(b) If $\varphi \neq 0$, then x is an eigenvalue of $H = H_0 + V$ as an operator on L^2.

Proof The argument is very similar to the proof of (a) of Theorem XIII.33. By the formula

$$(H_0 - x - i0)^{-1} = (H_0 + 1)^{-1} + (x + 1)(H_0 + 1)^{-1}(H_0 - x - i0)^{-1}$$

we see that $\psi \in (H_0 + 1)^{-1}[L^2_{-\delta}]$ so that $W\psi \in L^2_{-\delta}$ by Lemma 1. As a result, the integral $\int V(\xi)|\psi(\xi)|^2\, d\xi = (\rho^{-\delta}\psi, \rho^{-\delta}W\psi)$ is absolutely convergent and obviously real. But $V\psi = -\varphi$ so we conclude that $(\varphi, (H_0 - x - i0)^{-1}\varphi)$ is real. By Lemma 7, part (b), $\hat{\varphi} \restriction S_{x^{1/2}} \equiv 0$. As a result, Theorem IX.41 is applicable and we have the following "bootstrap" argument: Let $\delta = \frac{1}{2} + \varepsilon$. Since $\varphi \in L^2_\delta$, $\psi \in L^2_{\delta-1-\varepsilon}$ by Theorem IX.41. Using Lemma 1 and

$$W\psi = W(H_0 + 1)^{-1}\varphi + (x + 1)W(H_0 + 1)^{-1}\psi$$

we see that $W\psi \in L^2_{\delta-1-\varepsilon}$ also. Thus $\varphi = -V\psi = -\rho^{2\delta}W\psi$ is in $L^2_{\delta-1-\varepsilon+2\delta} = L^2_{\delta+\varepsilon}$. By this argument we have improved the estimate $\varphi \in L^2_\delta$ to $\varphi \in L^2_{\delta+\varepsilon}$. There is nothing to stop us from repeating it! Thus, $\varphi \in L^2_{\delta+n\varepsilon}$ for all n so $\psi \in L^2_{\delta-1+(n-1)\varepsilon}$ for all n. In particular $\psi \in L^2$. For $\eta \in \mathscr{S}$,

$$(H_0\eta, \psi) = \lim_{y \downarrow 0} (\eta, H_0(H_0 - x - iy)^{-1}\varphi) = \lim_{y \downarrow 0} (\eta, (x + iy)\psi + \varphi) = (\eta, x\psi + \varphi)$$

Therefore, $\psi \in D(H_0)$ and $H_0\psi = x\psi + \varphi = x\psi - V\psi$ so x is an eigenvalue of H as an operator on L^2. ∎

Completion of the proof of Theorem XIII.33 Choose $\delta > \frac{1}{2}$ so that $\rho^{2\delta}V = W$ is relatively H_0-compact. Given a compact subinterval $K \subset (0, \infty)\backslash\mathscr{E}_+$, consider the operator-valued function $A(\mu) = V(H_0 - \mu)^{-1}$ on $K \times [0, 1]$ where $(H_0 - \mu)^{-1}$ is interpreted as $(H_0 - x - i0)^{-1}$ if $\operatorname{Im} \mu = 0$. Then $A(\mu)$ is a function with values in the compact operators on L^2_δ, continuous on $K \times [0, 1]$ and analytic in its interior. Moreover, $A(\mu)\varphi = -\varphi$ has no nonzero solutions for $\mu \in K \times [0, 1]$. When $\operatorname{Im} \mu = 0$, this follows from the hypothesis $K \cap \mathscr{E}_+ = \varnothing$ and Lemma 8. For $\operatorname{Im} \mu \neq 0$, this follows from the facts that $(1 + V(H_0 - \mu)^{-1})(H_0 - \mu) = H - \mu$ and that both $H_0 - \mu$ and $H - \mu$ are invertible as maps of L^2_δ to L^2_δ by Lemma 1. It follows by a simple extension of the analytic Fredholm theorem (Theorem VI.14) that $(1 + A(\mu))^{-1}$ is a continuous function on $K \times [0, 1]$; in particular, it is uniformly bounded. But for $\operatorname{Im} \mu \neq 0$, $(H - \mu)^{-1} = (H_0 - \mu)^{-1} \times (1 + A(\mu))^{-1}$. Since $(H_0 - \mu)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ by Lemma 5 and $(1 + A(\mu))^{-1}$ is uniformly bounded from L^2_δ to L^2_δ, $(H - \mu)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ for $\mu \in K \times [0, 1]$. This is just a rephrasing of (b). ∎

* * *

Section XIII.6 Our discussion of what we call the Aronszajn-Donoghue theory closely follows that in W. F. Donoghue, "On the perturbation of spectra," *Comm. Pure Appl. Math.* **18** (1965), 559-579, who remarks that his results are essentially contained in N. Aronszajn, "On a problem of Weyl," *Amer. J. Math.* **79** (1957), 597-610. D. Pearson has found $V \in C^\infty$, $D^jV \to 0$ at $\pm\infty$ so that $-D^2 + V$ has purely singular continuous spectrum.

Section XIII.7 The theory of smooth operators was developed by T. Kato in two remarkable papers, "Wave operators and similarity for some non-self-adjoint operators," *Math. Ann.* **162** (1966), 258-279, and "Smooth operators and commutators," *Studia Math.* **31** (1968), 535-546. In the first paper Kato defined "H-smooth" and proved Theorems XIII.22 (in a stronger form; see Problem 49), XIII.23 (implicitly), XIII.24, XIII.25, XIII.26 (in a stronger form; see Problems 53, 54 and the discussion below), and XIII.27 (in the case $N = 2$). The second paper contains a criterion for H-smoothness if H is bounded—in case H is multiplicity free, this is the criterion of Example 4 and Problem 50—and Kato's proof of the Putnam-Kato theorem (Theorem XIII.28). Our proofs of these results are patterned on Kato's arguments.

What we call Kato's smoothness theorem appears in a stronger form in his *Math. Ann.* paper. First, he proves that $H_0 + \lambda V$ and H_0 are similar, i.e., $W(H_0 + \lambda V)W^{-1} = H_0$ for an invertible bounded operator W even when λ is complex. His proof is based on a "time-independent" formulation of scattering. Second, neither H_0 or V need be self-adjoint. What is important is that $\sigma(H_0) \subset \mathbb{R}$ and $|V|^{1/2}$ be H_0-smooth and H_δ^*-smooth in the sense of the basic definition (rather than the equivalent formulations in Theorem XIII.25) and that $\sup_{\mu \notin \mathbb{R}} \| |V|^{1/2}(H_0 - \mu)^{-1}|V|^{1/2}\| < \infty$.

Weak coupling results proving that $-\Delta$ and $-\Delta + V$ are unitarily equivalent for a suitable class of small V first appeared in J. Schwartz, "Some non-self adjoint operators," *Comm. Pure Appl. Math.* **13** (1960), 609-639. Schwartz dealt with the (reduced) two-body case in $\mathbb{R}^m$ with $m \geq 3$ and proved that if $\int (1 + x^2)|D^\alpha V|\, dx < \infty$ for all $\alpha \leq m - 1$, then $-\Delta$ and $-\Delta + \lambda V$ are unitarily equivalent for λ small.

Using the Dyson series (see Section X.12), R. Prosser proved a weak coupling theorem in the two-body case in "Convergent perturbation expansions for certain wave operators," *J. Mathematical Phys.* **5** (1964), 708–713. Kato proved Theorem XIII.27 in the case $N = 2$ in his *Math. Ann.* paper; in particular, (43) was used by Kato. The Prosser and Kato proofs are based on using the series

$$\Omega^- = 1 + i\int_0^\infty V_{s_1}\, ds_1 + i^2\int_0^\infty\int_0^{s_1} V_{s_2}V_{s_1}\, ds_2\, ds_1 + \cdots$$

where

$$V_s = e^{iH_0 s}Ve^{-iH_0 s}$$

for $\Omega^-\varphi$, and the norm estimate

$$\|V_{s_1}V_{s_2}\cdots V_{s_n}\varphi\| = \||V|^{1/2}\|\,\|V|^{1/2}e^{i(s_2-s_1)H_0}|V|^{1/2}\|\cdots\||V|^{1/2}e^{-is_nH_0}\varphi\|$$

Small coupling results for three-body problems were proven by Hunziker in his Boulder Lectures (see the Notes to Section XI.5) who used Prosser's techniques. He remarked that the techniques could not work for N-body systems with $N \geq 4$ because $\||V_{ij}|^{1/2}e^{isH_0}|V_{kl}|^{1/2}\|$ is constant if i, j, k, l are all distinct. The idea of controlling $\int |V_{ij}|^{1/2}e^{isH_0}|V_{kl}|^{1/2}\, ds$ which appears under "Case (3)" in our proof of Theorem XIII.27 and thereby the N-body results if $N \geq 4$ is due to R. Iorio and M. O'Carroll, "Asymptotic completeness for multi-particle Schrödinger Hamiltonians with weak potentials," *Comm. Math. Phys.* **27** (1972), 137–145. It is an open conjecture that the conclusion of Theorem XIII.27 holds if $V_{ij} \in L^{n/2}$.

The theorem that H has purely absolutely continuous spectrum if there exists an A with $i[H, A] \geq 0$ appeared first in C. R. Putnam, *Commutation Properties of Hilbert Space Operators and Related Topics*, Springer-Verlag, Berlin and New York, 1967. The proof we give is from Kato's *Studia* paper.

Application of the Kato–Putnam theory to repulsive potentials appeared first in R. Lavine, "Absolute continuity of Hamiltonian operators with repulsive potentials," *Proc. Amer. Math. Soc.* **22** (1969), 55–60. The theory was much further developed (and in particular Theorems XIII.29 and XIII.32 appear) in R. Lavine, "Commutators and scattering theory, I. Repulsive interactions," *Comm. Math. Phys.* **20** (1971), 301–323. Theorem XIII.29 appears in a slightly weaker form (an extra condition that $r\,\partial V/\partial r \ll H_0$ is added). For potentials, repulsive, central, and only $O(r^{-1-\epsilon})$, Lavine has proven the analogue of Theorem XIII.32 in "Completeness of the wave operators in the repulsive N-body problem," *J. Mathematical Phys.* **14** (1973), 376–379. Additional discussion of the two-body repulsive case can be found in M. Arai, "Absolute continuity of Hamiltonian operators with repulsive potentials," *Publ. Res. Inst. Math. Sci.* **7** (1971/72), 621–635. Our proof that $i[A, H_0] \geq 0$ follows Arai's paper.

Theorem XIII.31 and the notion of "H-smooth on Ω" are taken from R. Lavine, "Commutators and scattering theory, II. A class of one-body problems," *Indiana Univ. Math. J.* **21** (1972), 643–656.

The theory of smooth perturbations has been applied to the existence of propagators and scattering theory by E. B. Davies, "Time dependent scattering theory," *Math. Ann.* **210** (1974), 149–162, and extended to a Banach space setting in D. E. Evans, "Smooth perturbations in non-reflexive Banach spaces," *Math. Ann.* **221** (1976), 183–194.

Section XIII.8 Theorem XIII.33 is due to S. Agmon. He announced his results in "Spectral properties of Schrödinger operators," *Proc. Int. Cong. Math. of 1970*, Vol. 2, pp. 679–684, Gauthier-Villars, Paris, 1971. The details appear in S. Agmon, "Spectral properties of Schrödinger operators and scattering theory," *Ann. Scuola Norm. Sup. Pisa Cl. Sci.* **II**, 2 (1975), 151–218.

Our approach is based on a series of lectures by Agmon together with helpful remarks by H. Epstein, J. Ginibre, and R. Lavine. Theorem XIII.33d was proven prior to Agmon in T. Kato and S. Kuroda, "Theory of simple scattering and eigenfunctions expansions" in *Functional Analysis and Related Fields*, Springer-Verlag, Berlin and New York, 1970, 99–131. That (d) follows from Agmon's a priori estimates and the theory of local smoothness is a remark of R. Lavine in the paper quoted below.

Agmon's work represents the culmination of several lines of development. The first involves proving that $\sigma_{\text{sing}}(-\Delta + V) = \varnothing$ when V is $O(|x|^{-\mu})$ at ∞ (some of the papers quoted below require additional smoothness conditions). The earliest result was for $\mu > 2$ in the paper of Ikebe quoted in the Notes to Section XI.6. This was successively improved to $\mu > \frac{3}{2}$ by W. Jäger, "Zur Theorie der Schwingungsgleichung mit variablen Koeffizienten in Aussengebieten," *Math. Z.* **102** (1967), 62–88, to $\mu > \frac{4}{3}$ in P. Rejto, "On partly gentle perturbations, III" *J. Math. Anal. Appl.* **27** (1969), 21–67, to $\mu > \frac{5}{4}$ in T. Kato, "Some results on potential scattering," *Proc. Int. Conf. on Functional Analysis and Related Topics*, Tokyo, 1969, 206–215, and to $\mu > \frac{6}{5}$ by P. Rejto in "Some potential perturbations of the Laplacian," *Helv. Phys. Acta* **44** (1971), 708–736, and by S. Kuroda (quoted below). Rejto and Kuroda both modified their methods in response to Agmon's bootstrap argument and were able to handle all $\mu > 1$. Shortly after Agmon, and independently, the case $\mu > 1$ was handled by Y. Saito, "The principle of limiting absorption for second-order differential equations with operator-valued coefficients," *Pub. Res. Inst. Math. Sci.* **7** (1972), 581–619.

A second line of development involved the idea of proving $\sigma_{\text{sing}} = \varnothing$ by a perturbation theory of maps from X to X^* where X is a Banach space imbedded in $\mathscr{H}$. We discuss such an idea in the appendix to Section XI.6. This idea was developed by J. S. Howland, "Banach space techniques in the perturbation theory of self-adjoint operators with continuous spectra," *J. Math. Anal. Appl.* **20** (1967), 22–47, and "A perturbation-theoretic approach to eigenfunction expansions," *J. Functional Analysis* **2** (1968), 1–23, and by P. A. Rejto, "On partly gentle perturbations, I–III," *J. Math. Anal. Appl.* **17** (1967), 435–462; **20** (1967), 145–187; **27** (1969), 21–67. The use of weighted L^2 spaces was first advocated (in a slightly different context) by S. Kuroda, "On the Hölder continuity of an integral involving Bessel functions," *Quart. J. Math. Oxford Ser.* **21** (1970), 71–81.

A third line of development involved the abstract theory of eigenfunction expansions of Kuroda (see the Notes to Section XI.6) and the theory of higher order elliptic operators. In fact, Agmon's theory works for a large class of operators (see Problem 70 and below). A theory with similar results was developed (partly independently of Agmon) by S. Kuroda in "Scattering theory for differential operators, I, II," *J. Math. Soc. Japan* **25** (1973), 75–104; 222–234. Let $H_0 = \sum_{|\alpha|\leq 2m} a_\alpha(-iD)^\alpha$ where a_α is real. Suppose moreover that H_0 is **elliptic**, that is, $\sum_{|\alpha|=2m} a_\alpha k^\alpha \neq 0$ for all $k \in \mathbb{R}^n$, $k \neq 0$. Let $P_1(k) = \sum_{|\alpha|\leq 2m} a_\alpha k^\alpha$. A point k where grad $P_1 = 0$ is called a critical point and the value of P_1 at such a point is called a **critical value**. It can be shown that H_0 has only finitely many critical values λ_i. Let $V = \sum_{|\alpha|\leq 2m} V_\alpha(x)(-iD)^\alpha$ be such that: (i) $|V_\alpha(x)| \leq C_\alpha(1 + |x|^2)^{-1/2-\epsilon}$. (ii) V is formally self-adjoint, i.e., $(\varphi, V\varphi)$ is real for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$. (iii) For each $x \in \mathbb{R}^n$ and $k \in \mathbb{R}^n\backslash\{0\}$, $\sum_{|\alpha|=2m}(a_\alpha + V_\alpha(x))k^\alpha \neq 0$. Then Agmon and Kuroda have proven the following generalization of Theorem XIII.33:

(a) The eigenvalues of $H_0 + V$ at noncritical values of H_0 are of finite multiplicity and can have only critical values of H_0 as limit points.

(b) If $[a, b]$ is disjoint from all critical values of H_0 and all eigenvalues of $H \equiv H_0 + V$ and if $\delta > \frac{1}{2}$, then

$$\sup_{a\leq x\leq b;\, 0<y<1} \|(H - x - iy)^{-1}\|_{\delta,-\delta} < \infty$$

(c) $\sigma_{sing}(H_0 + V) = \varnothing$.
(d) Wave operators exist and are complete.

Extensions of the Agmon-Kuroda work to a slightly larger class of potentials can be found in S. Agmon and L. Hormander, "Asymptotic properties of solutions of differential equations with simple characteristics," *J. Anal. Math.* **30** (1976), 1-38. These authors use slightly different spaces which they consider more natural.

In Agmon's original work, he does not prove or use the existence of limiting boundary values for $(H_0 - \lambda)^{-1}$ or $(H - \lambda)^{-1}$. Lemmas 6 and 7 were replaced by a limiting argument known as the "principle of limiting absorbtion." The quadratic estimates of Lemma 6 are due to Lavine.

Theorem XIII.33 is capable of generalization in two other directions. First, V need only be form compact (see Problem 71). Secondly, one can discuss the case $V = V_1 + V_2$ where $\partial V_1/\partial r$ and V_2 are $O(r^{1-\varepsilon})$ at ∞. This is done by R. Lavine, "Absolute continuity of positive spectrum for Schrödinger operators with long range potentials," *J. Functional Analysis* **12** (1973), 30-54. See also T. Ikebe and Y. Saito, "The limiting absorbtion method and absolute continuity for the Schrödinger operator," *J. Math. Kyoto* **12** (1972), 513-542, and Y. Saito, "The principle of limiting absorbtion for the non-self-adjoint Schrödinger operator in $\mathbb{R}^n (N \neq 2)$" *Publ. Res. Inst. Math. Sci.* **9** (1974), 397-428.

Further developments of the Agmon-Kuroda theory appear in a series of papers by M. Schechter, "A unified approach to scattering," *J. Math. Pures Appl.* **53** (1974), 373-396; "Scattering theory for elliptic operators of arbitrary order," *Comm. Math. Helv.* **49** (1974), 84-113; "Scattering theory for second order elliptic operators," *Ann. Mat. Pura et Appl.* **55** (1975), 313-331, "Scattering Theory for Elliptic Systems," *J. Math. Soc. Japan* **28** (1976), 71-79; and "Nonhomogeneous elliptic systems and scattering," *Tohoku Math. J.* **27** (1975), 601-616.

The Agmon method has been extended to study $-\Delta + V + \mathbf{a} \cdot \mathbf{x}$ in I. W. Herbst, "Unitary equivalence of Stark Hamiltonians," *Math. Z.* **155** (1977), 55-71. Herbst proves that if $V = V_1 + V_2$ where $V_2 \in L^2(\mathbb{R}^3)$ has compact support, V_1 satisfies $|V_1(x)| \leq C(1 + (\mathbf{a} \cdot \mathbf{x})^2)^{-1/4-\varepsilon}$, and $-\Delta + V + \mathbf{a} \cdot \mathbf{x}$ has no eigenvalues, then $\Omega^{\pm}(-\Delta + V + \mathbf{a} \cdot \mathbf{x}, -\Delta + \mathbf{a} \cdot \mathbf{x})$ exist and are unitary. Avron and Herbst, in their paper quoted in the notes to Section 4, give criteria under which $-\Delta + V + \mathbf{a} \cdot \mathbf{x}$ has no eigenvalues.

* * *

47. (a) Suppose the basic smoothness estimate (31) holds for a dense set of φ. Prove that for any φ, $R(\lambda \pm i\varepsilon)\varphi \in D(A)$ a.e. in λ (ε fixed, $\varepsilon \neq 0$) and that (31) holds.
(b) Suppose that for a fixed $\varepsilon > 0$, $\int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2 \, d\lambda < \infty$ for each $\varphi \in \mathscr{H}$. Prove that

$$\int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2 \, d\lambda \leq C\|\varphi\|^2$$

for some C and all φ. (Hint: Apply the closed graph theorem to the map $\varphi \mapsto AR(\lambda + i\varepsilon)\varphi$ of $\mathscr{H}$ into $L^2(\mathbb{R}, d\lambda; \mathscr{H})$.)
(c) Suppose that $\sup_{\varepsilon > 0} \int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2 \, d\lambda < \infty$ for each φ. Prove that A is H-smooth. (Hint: Use (b) and the uniform boundedness principle.)

48. Let f be a bounded Borel function on $\mathbb{R}$ and suppose $f(H)$ is H-smooth for some self-adjoint operator H. Prove that $f(H) = 0$.

49. (a) Let H be self-adjoint and let A be H-smooth. Prove that A is $|H|^{\alpha}$-bounded for any $\alpha > \frac{1}{2}$. (Hint: Use form (3) of Theorem XIII.25 to prove that $(H^2 + 1)^{-\alpha/2} A^*$ is bounded.)

(b) Let $H = -i \, d/dx$ on $L^2(\mathbb{R})$. Prove that there exist $\varphi \in Q(H)$ that are not bounded.
(c) Find an H-smooth operator A so that A is not $|H|^{1/2}$-bounded. (Hint: Use Example 1.)

50. Let H be multiplication by x on $L^2([\alpha, \beta], dx)$ with $\alpha, \beta \in \mathbb{R}$. Suppose that A is bounded and A^*A has integral kernel K. Prove that $\|A\|_{HS}^2 \equiv \|K\|_1$.

**51.* Let H be multiplication by x on $L^2([\alpha, \beta], dx)$ with $\alpha, \beta \in \mathbb{R}$. Suppose that A is bounded and H-smooth. Prove that A^*A has the form (37). (Hint: First show that A^*x is in L^1 for every x with $\|A^*x\|_1 \leq C\|x\|_2$ and then use the Dunford-Pettis theorem (Problem 33 in Chapter V) to find a bounded measurable function F from $[\alpha, \beta]$ to $\mathscr{H}$, so that $(A^*x)(\lambda) = (F(\lambda), x)$.
Reference for Problem 51: Kato's *Studia Math.* paper (see the Notes to Section 7).

52. Let A and B be self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. Suppose C is A-smooth and D is a bounded operator on $\mathscr{H}_2$. Prove that $C \otimes D$ is $A \otimes I + I \otimes B$-smooth.

53. Under the hypotheses of Theorem XIII.26, prove that for any $\lambda \in \mathbb{C}$ with $|\lambda| \leq 1$, $H_0 + \lambda \sum_{i=1}^{n} C_i$ is a strictly m-accretive form on $Q(H_0)$, and that the associated operator H has $\sigma(H) \subset \sigma(H_0)$ and obeys $\sup \| |C_i|^{1/2} (H - z)^{-1} |C_j|^{1/2} \| < \infty$ for all i, j (continued in the next problem).

**54.* (continued from Problem 53) Let $R(\mu)$ be the resolvent of H_0 and $R(\mu; \lambda)$ the resolvent of $H(\lambda) = H_0 + \lambda \sum_{i=1}^{n} C_i$. Define $W^{\pm}(\lambda)$ by

$$(\varphi, W_{\pm}(\lambda)\psi) = (\varphi, \psi) \mp \frac{\lambda}{2\pi i} \sum_{i=1}^{n} \int_{-\infty}^{\infty} (C_i^{1/2} R(\mu \pm i0)\varphi, \, |C_i|^{1/2} R(\mu \mp i0, \lambda)\psi) \, d\mu$$

Prove that
(a) $W_{\pm}(\lambda)$ are analytic in the region $|\lambda| \leq 1$.
(b) $W_{\pm}(\lambda)$ are invertible and $H(\lambda) = W_{\pm}(\lambda) H_0 W_{\pm}(\lambda)^{-1}$.
(c) If λ is real, $W^{\pm}(\lambda) = \Omega^{\pm}(\lambda)$.

55. Let A and H_0 be self-adjoint operators with $\mathrm{Ker}(A) = \{0\}$. Prove that, for any positive integers $n \neq m$, at most one of A^n and A^{-m} is H_0 smooth.

56. Let $V \in R$, the Rollnik class, with $\|V\|_R < 4\pi$. Prove that the wave operators provide unitary equivalences of $-\Delta$ and $-\Delta + V$ and in particular that scattering is complete.

57. (a) Let $H_n = H_0 + A_n^* B_n$ where B_n is H_0-smooth and A_n is H_n-smooth. Suppose that $\sup_n \|A_n\|_{H_n} < \infty$ and $\lim_{n \to \infty} \|B_n\|_{H_0} = 0$. Prove that $\Omega_n^{\pm} \equiv \text{s-lim}_{t \to \mp\infty} e^{itH_n} e^{-itH_0}$ converges to 1 *in norm*. In particular verify the norm continuity of $\Omega^{\pm}(\lambda) = \text{s-lim}_{t \to \mp\infty} e^{it(H_0 + \lambda C)} e^{-itH_0}$ for $\lambda \in (-1, 1)$, in the context of Theorem XIII.26.
(b) Let $V_n \to V$ in Rollnik norm. Prove that the corresponding S matrices converge strongly. (Hint: Write $V_n = W_n + Y_n$, $V = W + Y$, so that $Y_n \to Y$ in $L^1 \cap R$, $W_n \to W$ in R, and $\sup_n \|W_n\|_R < 4\pi$.)

58. (a) Let H_0 be the operator on $L^2[0, \infty)$ that is the closure of $-d^2/dx^2$ on $\{u \in C_0^{\infty}[0, \infty) \mid u(0) = 0\}$. Let $E \notin \sigma(H_0)$ and let

$$K_E(x, y) = E^{-1/2} \sin[\sqrt{E} \min\{x, y\}] \exp[i\sqrt{E} \max\{x, y\}]$$

where $\sqrt{E}$ is the square root with $\operatorname{Im}\sqrt{E} > 0$. Prove that

$$[(H_0 - E)^{-1}\varphi](y) = \int_0^\infty K_E(x, y)\varphi(y)\, dy$$

(b) $|K_E(x, y)| \le \sqrt{xy}$.

(c) Let V be a measurable function on $[0, \infty)$ with $\int_0^\infty x|V(x)|\, dx < \infty$. Then,

$$\sup_{E \notin \mathbb{R}} \| |V|^{1/2}(H_0 - E)^{-1}|V|^{1/2}\| < \infty$$

(d) If $\int_0^\infty x|V(x)|\, dx < 1$, then H_0 and $H_0 + V$ are unitarily equivalent and the wave operators are unitary equivalences.

59. Let A and H be bounded self-adjoint operators and let $R(\mu) = (H - \mu)^{-1}$. Prove that

$$|\varepsilon|\,|(R(\lambda + i\varepsilon)\varphi, [H, A]R(\lambda + i\varepsilon)\varphi)| \le \|A\|\,\|\varphi\|^2$$

and use this to prove that $(i[H, A])^{1/2}$ is H-smooth if $i[H, A] \ge 0$.

60. Let A and B be bounded self-adjoint operators and c a strictly positive real number. Prove that $i[A, B] \ge cI$ is impossible by:
(a) using the theory of smooth perturbations;
(b) direct computation (look at $e^{iAt}Be^{-iAt}$).

61. Extend the Kato-Putnam theorem to the case where H is unbounded and $i[H, A] > 0$ means that $i(A\varphi, H\varphi) - i(H\varphi, A\varphi) > 0$ for all $\varphi \in D(H)$, $\varphi \neq 0$.

†62. Suppose that $f(t)$ is a Banach-space-valued uniformly continuous function on $\mathbb{R}$. Suppose also that $\int_{-\infty}^{\infty} \|f(t)\|^p\, dt < \infty$ for some $p < \infty$. Suppose that f is strongly differentiable with a uniformly bounded derivative. Conclude that $\lim_{t\to\pm\infty} f(t) = 0$.

†63. Fill in the computations in the proof of Theorem XIII.29.

†64. Fill in the details of the proof of Theorem XIII.32.

65. By iterating the proof of (a) in Theorem XIII.33, prove that if $H_0\varphi = \lambda\varphi - V\varphi$ with $\lambda > 0$, then $\varphi \in L^2_\delta$ for all δ.

†66. (a) Prove that $(-\Delta - \mu)^{-1}$ is bounded from L^2_δ to L^2_δ for any δ and any $\mu \in \mathbb{C}\backslash\mathbb{R}$. (Hint: Prove it for $\delta > 0$ inductively in $[0, 1], (1, 2], \ldots$.)
(b) Complete the proof of Lemma 1 in Section 8.
(c) Prove that $(-\Delta + 1)^{-1}\,\partial/\partial x_i$ is a bounded map from L^2_δ to L^2_δ for any δ.

†67. Verify the bound (62).

68. Let $\delta > n + \frac{1}{2}$. Prove that, for any $b > a > 0$, there is a constant C so that

$$\|(-\Delta - \lambda - i0)^{-n}\varphi\|_{-\delta} \le C\|\varphi\|_\delta$$

for all $\varphi \in \mathscr{S}(\mathbb{R}^m)$ and all $\lambda \in [a, b]$.

69. Let $\|A\|_{\delta,-\delta}$ denote the norm of A as a map of L^2_δ to $L^2_{-\delta}$. Let $\delta > \frac{1}{2}$. Prove that for any $\alpha < \min\{1, \delta - \frac{1}{2}\}$, $(H_0 - \mu - i0)^{-1}$ is Hölder continuous of order α as an $\mathscr{L}(L^2_\delta, L^2_{-\delta})$-valued function of μ, i.e., for any $\mu > 0$, there is a C and an ε so that

$$\|(H_0 - \mu' - i0)^{-1} - (H_0 - \mu - i0)^{-1}\|_{\delta,-\delta} \le C|\mu - \mu'|^\alpha$$

if $|\mu - \mu'| < \varepsilon$.

*70. Let V be an Agmon potential. Let $a_1, \ldots, a_n$ obey $\sum_{i=1}^n \partial_j a_j = 0$ (distributional sense) with $|a_j(x)| \le C_j(1 + |x|^2)^{-1/2-\varepsilon}$. Let

$$H = -\Delta + 2i\sum_{j=1}^n a_j\,\partial_j + \sum_{j=1}^n a_j^2 + V$$

Prove that $\sigma_{\text{sing}}(H) = \varnothing$ and that $\Omega^\pm(H, H_0)$ exist and are complete. (Hint: Develop a theory paralleling Theorem XIII.33.)

*71. Suppose $V(x) = (1 + |x|^2)^{-1/2-\varepsilon}W(x)$ where W is a form relatively compact perturbation of $-\Delta$. Prove that Theorem XIII.33 remains valid.

List of Symbols

Superscripts refer to page numbers in other volumes. The boldface convention is discussed on page 7.

$\mathbf{C}$	the complex numbers	
$C(X)$		102^1
$C_0^\infty(\mathbf{R}^n)$		145^1
$\mathscr{C}_{\alpha,\beta}$		96
$d\Gamma(A)$		302^1, 208^2
$\mathscr{D}_{L^\infty}$		67
$D(\cdot)$	(domain)	249^1
$\mathscr{D}(\mathbf{R}^n)$, $\mathscr{D}(\Omega)$		147^1
$\mathscr{D}'(\mathbf{R}^n)$, $\mathscr{D}'(\Omega)$		148^1
D^α		2^2
$D(\alpha)$		84
$D \lhd D'$		89
$D' * D$		91
EBFM		4
$\mathscr{E}$		99
$E_\Omega(A)$		28
$f(k)$		117
$f(k, \theta)$		111
$f(E, \cos\theta)$		127
$f(A)$	(continuous functional calculus)	222^1
$\hat{f}$, $\mathscr{F}$	(Fourier transform)	1^2
$\check{f}$, $\mathscr{F}$	(inverse Fourier transform)	1^2
$\mathscr{F}(\mathscr{H})$		53^1
$F_\perp(x)$		175
$F_\parallel(x)$		175
$G_0(x, y)$		102, 103
$G(x, y)$		102, 103
$G_{\Gamma;D}$		206
$G_{\Gamma;N}$		206
$\mathscr{H}$		295
$\mathscr{H}$		39^1
$\mathscr{H}_{pp}$, $\mathscr{H}_{ac}$, $\mathscr{H}_{sing}$		230^1
$\mathscr{H}_{asym}$		85
$\mathscr{H}_e$		85
$\mathscr{H}_\pm^2$		219
$\mathscr{H}_{\substack{in \\ out}}$		321
H_0	(free Hamiltonian)	55^2
H_e		85
H_{asym}		85
$H^\otimes$		290
$H(C_\ell)$, $\tilde{H}(C_\ell)$		79

H_D 79
$\mathscr{I}_p$ 207^1, 208^1, 41^2, 47
$\mathscr{I}_p(\mathscr{H}_1, \mathscr{H}_2)$ 36
I_D 79
Ker 185^1
KLMN 167^2
ℓ_p 69^1
$L^p(X, d\mu)$ 68^1
$L^2(X, d\mu : \mathscr{H}')$ 40^1
L^p_{loc} (functions locally L^p)
L^2_δ (weighted L^2) 47
L^p_w (weak L^p) 30^2
$L^r + L^s$ 165^2
$\mathscr{L}(\mathscr{H})$ 182^1
$\mathscr{L}(X, Y)$ 69^1
$\mathscr{M}(B)$ 23
$p(D)$ 45^2
$P_\Omega(A)$, P^A_Ω 234^1
P_{cont} 341
$\mathscr{P}_n$ 323
$\mathbb{R}$ the real numbers
R (Rollnik class) 99
$R_{\alpha\beta}$ 95
Ran 185^1
$R(\lambda + i\mu)$, $R_\lambda(T)$ (resolvent) 188^1
R_0, $R_{\Gamma;N}$, $R_{\Gamma;D}$, $\tilde{R}_{\partial B \cup \Gamma;N}$ 203
supp 139^1, 17^2
S (scattering operator) see index
$\hat{S}$, $\tilde{S}$ 213
$S(E)$ 123
$S(k, k')$ 108
$\mathscr{S}(\mathbb{R}^n)$ 133^1
$\mathscr{S}'(\mathbb{R}^n)$ 134^1
$\mathrm{tr}(\cdot)$ 207^1, 208^1
TVEV 323
$T(k, k')$ 107
$T(E)$ 127
VEV 323
$W_m(\Omega)$ (Sobolev spaces) 50^2
x^α 2^2
$\Gamma(T)$ (operator graph) 250^1
$\Gamma(A)$ 309^1, 208^2
$d\Gamma(A)$ 302^1, 208^2
$\delta_\ell(E)$ 129
Δ (symmetric set difference)
Δ (Laplacian on $\mathbb{R}^n$)
Δ^Ω_D (Dirichlet Laplacian) 263^4
Δ^Ω_N (Neumann Laplacian) 263^4
$\kappa(X)$ 111^1
$\rho(T)$ 188^1
$\sigma(T)$ 188^1
σ_x, σ_y, σ_z, $\sigma_\pm$ (Pauli matrices) 287
σ_{pp}, σ_{cont}, σ_{ac}, σ_{sing} 231^1
σ_{disc} 236^1
σ_{ess} 236^1, 15
σ (cross section) 15, 111
$d\sigma/d\Omega$ (differential cross section) 15
Σ_{in}, Σ_{out} 3
Σ_0 8
$\tau_F(k)$ 116
$\hat{\mathscr{F}}$ 86
$\mathscr{T}_\alpha$ 85
χ_A 2^1
$\Omega^\pm$ 8
$\Omega^\pm(A, B)$ 17
$\Omega^\pm(A, B, J)$ 24
$\Omega^\pm_\alpha$ 85
$\|\cdot\|_p$ (functions) 68^1
$\|\cdot\|_p$ (operators) 41^2
$\|\cdot\|_R$ (Rollnik norm) 99
$\|\cdot\|_\infty$ (functions) 67^1
$\|\cdot\|_\infty$ (operators) 81^2
$\|\cdot\|_\delta$ (weighted L^2) 438
$\|\cdot\|_{op}$ (operator norm) 9^1
$\oplus$ 40^1, 78^1
$\otimes$ (measures) 26^1
$\otimes$ (Hilbert spaces) 49^1
$\otimes$ (functions) 141^1
$\otimes$ (operators) 299^1
$\leq$ (operators) 75^4, 85^4, 269^4
$\lhd$ 89
$\bar{\ }$ (closure) 92^1
$^\circ$, ^{int} (interior) 92^1
* (adjoint) 187^1
* (dual space) 72^1
* (convolution) 6^2, 7^2
* (common cluster refinement) 91
$\xrightarrow{\|\cdot\|}$, $\xrightarrow{w}$, $\xrightarrow{s}$ 182^1, 183^1
$|\cdot|$ (absolute value of an operator) 196^1
$\perp$ (orthogonal complement) 41^1
$\setminus$ (set difference) 1^1
$/$ (quotient) 78^1, 79^1
$\restriction$ (restriction) 2^1
$\langle\cdot,\cdot\rangle$ (ordered pair) 1^1
$(\cdot,\cdot)$ (inner product) 36^1

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METHODS OF MODERN MATHEMATICAL PHYSICS

IV: ANALYSIS OF OPERATORS

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To David

To Rivka and Benny

Preface

. . . of making books there is no end, and much study is a weariness of the flesh
Koheleth (Ecclesiastes) 12:12

With the publication of Volumes III and IV we have completed our presentation of the material which we originally planned as "Volume II" at the time of publication of Volume I. We originally promised the publisher that the entire series would be completed nine months after we submitted Volume I. Well! We have listed the contents of future volumes below. We are not foolhardy enough to make any predictions.

We were very fortunate to have had T. Kato and R. Lavine read and criticize Chapters XII and XIII, respectively. In addition, we received valuable comments from J. Avron, P. Deift, H. Epstein, J. Ginibre, I. Herbst, and E. Trubowitz. We are grateful to these individuals and others whose comments made this book better.

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Introduction

Il libro della natura é scritto in lingua matematica. — *Galileo Galilei*

The first step in the mathematical elucidation of a physical theory must be the solution of the existence problem for the basic dynamical and kinematical equations of the theory. Once that is accomplished, one would like to find general qualitative features of these solutions and also to study in detail specific special systems of physical interest.

Having discussed the general question of the existence of dynamics in Chapter X, we present methods for the study of general qualitative features of solutions in this volume and its companion (Volume III) on scattering theory. We concentrate on the Hamiltonians of nonrelativistic quantum mechanics although other systems are also treated. In Volume III, the main theme is the long-time behavior of dynamics, especially of solutions which are "asymptotically free." In this volume, the main theme involves the five kinds of spectra defined in Sections VII.2 and VII.3: the essential spectrum, σ_{ess}; the discrete spectrum, σ_{disc}; the absolutely continuous spectrum, σ_{ac}; the pure point spectrum, σ_{pp}; and the singular continuous spectrum, σ_{sing}. It turns out that the study of the absolutely continuous spectrum as well as the problem of showing that the continuous singular spectrum is empty are intimately connected with scattering theory. Thus, the separation of the material in Volumes III and IV is somewhat artificial. For this reason, we preprinted in Volume III three sections from Volume IV.

These are not the only sections in which the themes of the two volumes overlap.

In these volumes specific systems are usually presented to illustrate the application of general mathematical methods, but the detailed analysis of the specific systems is not carried very far. Mathematical physicists have to some extent neglected the detailed study of specific systems; we believe that this neglect is unfortunate, for there are many interesting unsolved problems in specific systems, even in the purely Coulombic model of atomic physics. For example, it has not been shown that H^{--} has no bound states even though the analogous classical system of one positive and three negative charges has the property that its energy is lowered by moving a suitable electron to infinity. And it is not known rigorously that the energy needed to remove the first electron from an atom is less than the energy needed to remove the second, even though this is "physically obvious." We hope that by collecting the general mathematical methods in Volumes II, III, and IV, we have made the analysis of specific systems easier and more attractive.

Nonrelativistic quantum mechanics is often viewed by physicists as an area whose qualitative structure, especially on the level treated here, is completely known. It is for this reason that a substantial fraction of the theoretical physics community would regard these volumes as exercises in pure mathematics. On the contrary, it seems to us that much of this material is an integral part of modern quantum theory. To take a specific example, consider the question of showing the absence of the singular continuous spectrum and the question of proving asymptotic completeness for the purely Coulombic model of atomic physics. The former problem was solved affirmatively by Balslev and Combes in 1970, the latter is still open. Many physicists would approach these questions with Goldberger's method: "The proof is by the method of reductio ad absurdum. Suppose asymptotic completeness is false. Why that's absurd! Q.E.D." Put more precisely: If asymptotic completeness is not valid, would we not have discovered this by observing some bizarre phenomena in atomic or molecular physics? Since physics is primarily an experimental science, this attitude should not be dismissed out of hand and, in fact, we agree that it is extremely unlikely that asymptotic completeness fails in atomic systems. But, in our opinion, theoretical physics should be a science and not an art and, furthermore, one does not fully understand a physical fact until one can derive it from first principles. Moreover, the solution of such mathematical problems can introduce new methods of calculational interest (for example, Faddeev's treatment of completeness in three-body systems and the application of his ideas in nuclear physics) and can provide important elements of

clarity (for example, the physical artificiality of "adiabatic switching" in nonrigorous scattering theory and the clarifying work of Cook, Jauch, and Kato).

The general remarks about notes and problems in earlier introductions are applicable here with one addition: the bulk of the material presented in this volume is from advanced research literature, so many of the "problems" are quite substantial. Some of the starred problems summarize the contents of research papers!

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XII: Perturbation of Point Spectra

In the thirties, under the demoralizing influence of quantum-theoretic perturbation theory, the mathematics required of a theoretical physicist was reduced to a rudimentary knowledge of the Latin and Greek alphabets.

Res Jost

In this chapter we shall examine the following general situation: An operator H_0 has an eigenvalue E_0, which we usually assume is in the discrete spectrum. Suppose that H_0 is perturbed a little; that is, consider $H_0 + \beta V$ where V is some other operator and $|\beta|$ is small. What eigenvalues of $H_0 + \beta V$ lie near E_0 and how are they related to V? What are their properties as functions of β? Such a situation is familiar in quantum mechanics where there are *formal* series for the perturbed eigenvalues. These **Rayleigh–Schrödinger series** are not special to quantum-mechanical operators but exist for many perturbations of the form $H_0 + \beta V$. The heart of this chapter is the second section where we shall discuss the beautiful Kato–Rellich theory of regular perturbations; this theory gives simple criteria under which one can prove that these formal series have a nonzero radius of convergence. We then discuss what the perturbation series means in cases where it is divergent or not directly related to eigenvalues.

XII.1 Finite-dimensional perturbation theory

We first discuss finite-dimensional matrices. Not only will this allow us to present explicit formulas in the simplest case, but we shall eventually treat

degenerate perturbation theory by reducing it to an essentially finite-dimensional problem. Furthermore, an important difficulty already occurs in the finite-dimensional case, namely proving analyticity in β when there is a degenerate eigenvalue. Recall that E_0 is called a **degenerate eigenvalue** when the characteristic equation for H_0, $\det(H_0 - \lambda) = 0$, has a multiple root at $\lambda = E_0$. In an appendix to this section we review the theory of matrices with degenerate eigenvalues and, in particular, we discuss the Jordan normal form.

First consider the elementary example

$$T(\beta) = \begin{bmatrix} 1 & \beta \\ \beta & -1 \end{bmatrix}$$

By our definition of operator-valued analytic function in Section VI.3, $T(\beta)$ is a matrix-valued analytic function. To find its eigenvalues, we need only solve $\det(T(\beta) - \lambda) = 0$ (the **secular** or **characteristic equation**). Thus

$$\lambda_{\pm}(\beta) = \pm\sqrt{\beta^2 + 1}$$

are the eigenvalues. This problem has several characteristic features:

(i) Even though $T(\beta)$ is entire in β, the eigenvalues are not entire but have singularities as functions of β.

(ii) The singularities are not on the real β axis where $T(\beta)$ is self-adjoint but occur at nonreal β, namely at $\beta = \pm i$. Thus, while there are no singularities at "physical" values, the **perturbation series**, i.e., the Taylor series for $\lambda_{\pm}(\beta)$ at $\beta = 0$, have a finite radius of convergence due to complex singularities.

(iii) "Level crossing" takes place at the singular values of β; that is, at $\beta = \pm i$ there are fewer distinct eigenvalues, namely one, than at other points, where there are two.

(iv) At the singular values of β the matrix $T(\beta)$ is *not* diagonalizable. Explicitly

$$T(i)\begin{bmatrix} 2 \\ 2i \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad T(i)\begin{bmatrix} 1 \\ -i \end{bmatrix} = \begin{bmatrix} 2 \\ 2i \end{bmatrix}$$

so the matrix of $T(i)$ in the basis $\langle 2, 2i\rangle$, $\langle 1, -i\rangle$, is

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

While this "Jordan anomaly" is typical, we leave a discussion of it to the Notes; see also Problem 23.

(v) The analytic continuation of an eigenvalue is an eigenvalue.

For the remainder of this section, we shall suppose that $T(\beta)$ is a matrix-valued analytic function in a connected region R of the complex plane. Notice that we do not require $T(\beta)$ to be linear in β. Later, we shall be able to reduce the infinite-dimensional, linear, finitely degenerate perturbation problem to a finite-dimensional problem, but one that is no longer *linear* in β. Thus, greater generality at this point will be crucial.

To find the eigenvalues of $T(\beta)$ we must solve a secular equation

$$\det(T(\beta) - \lambda) = (-1)^n[\lambda^n + a_1(\beta)\lambda^{n-1} + \cdots + a_n(\beta)] = 0$$

The basic theorem about such functions is:

Theorem XII.1 Let $F(\beta, \lambda) = \lambda^n + a_1(\beta)\lambda^{n-1} + \cdots + a_n(\beta)$ be a polynomial of degree n in λ whose leading coefficient is one and whose coefficients are all analytic functions of β. Suppose that $\lambda = \lambda_0$ is a simple root of $F(\beta_0, \lambda)$. Then for β near β_0, there is exactly one root $\lambda(\beta)$ of $F(\beta, \lambda)$ near λ_0, and $\lambda(\beta)$ is analytic in β near $\beta = \beta_0$.

Proof This is a special case of the implicit function theorem. Since $F(\beta, \lambda)$ is analytic near β_0 and λ_0, we can write $F(\beta, \lambda) = \sum_{m=0}^{n} (\lambda - \lambda_0)^m f_m(\beta)$ with $f_0(\beta_0) \equiv F(\beta_0, \lambda_0) = 0$, and $f_1(\beta_0) \equiv (\partial F/\partial\lambda)(\beta_0, \lambda_0) \neq 0$ since λ_0 is a simple root. Thus to find solutions of $F(\beta, \lambda) = 0$, we need only solve the equivalent equation

$$\lambda = \lambda_0 - \frac{f_0(\beta)}{f_1(\beta)} - \sum_{m=2}^{n} (\lambda - \lambda_0)^m \frac{f_m(\beta)}{f_1(\beta)} \tag{1}$$

Because $f_1(\beta_0) \neq 0$, all the coefficients $f_k(\beta)/f_1(\beta)$ are analytic near $\beta = \beta_0$. We try to solve this last equation with a solution of the form $\lambda(\beta) = \lambda_0 + \sum_{k=1}^{\infty} \alpha_k(\beta - \beta_0)^k$. The α_k can be computed by recursive substitution into (1); for example,

$$\alpha_1 = -\left[\frac{f_0(\beta)}{f_1(\beta)}\right]' \Bigg|_{\beta=\beta_0}$$

and

$$\alpha_2 = -\frac{1}{2}\left[\frac{f_0(\beta)}{f_1(\beta)}\right]'' \Bigg|_{\beta=\beta_0} - \alpha_1^2 \frac{f_2(\beta_0)}{f_1(\beta_0)}$$

It is not very hard to prove that the α's determined recursively yield a power series with a nonzero radius of convergence (Problem 1a). Uniqueness is also fairly easy (Problem 1b). ∎

Corollary Let $T(\beta)$ be a matrix-valued analytic function near β_0 and suppose λ_0 is a simple eigenvalue of $T(\beta_0)$. Then:

(a) For β near β_0, $T(\beta)$ has exactly one eigenvalue, $\lambda_0(\beta)$, near λ_0.

(b) $\lambda_0(\beta)$ is a simple eigenvalue if β is near β_0.
(c) $\lambda_0(\beta)$ is analytic near $\beta = \beta_0$.

For multiple roots, a more complicated but still straightforward analysis is necessary. We do not prove the following basic theorem for this case (proofs can be found in the references in the Notes).

Theorem XII.2 Let $F(\beta, \lambda) = \lambda^n + a_1(\beta)\lambda^{n-1} + \cdots + a_n(\beta)$ be an nth degree polynomial in λ whose leading coefficient is one and whose coefficients are all analytic functions of β. Suppose $\lambda = \lambda_0$ is a root of multiplicity m of $F(\beta_0, \lambda)$. Then for β near β_0, there are exactly m roots (counting multiplicity) of $F(\beta, \lambda)$ near λ_0 and these roots are the branches of one or more multivalued analytic functions with at worst algebraic branch points at $\beta = \beta_0$. Explicitly, there are positive integers $p_1, \ldots, p_k$ with $\sum_{i=1}^{k} p_i = m$ and multivalued analytic functions $\lambda_1, \ldots, \lambda_k$ (not necessarily distinct) with convergent **Puiseux series** (Taylor series in $(\beta - \beta_0)^{1/p}$)

$$\lambda_i(\beta) = \lambda_0 + \sum_{j=1}^{\infty} \alpha_j^{(i)} (\beta - \beta_0)^{j/p_i}$$

so that the m roots near λ_0 are given by the p_1 values of λ_1, the p_2 values of λ_2, etc.

Corollary If $T(\beta)$ is a matrix-valued analytic function near β_0 and if λ_0 is an eigenvalue of $T(\beta_0)$ of algebraic multiplicity m, then for β near β_0, $T(\beta)$ has exactly m eigenvalues (counting multiplicity) near λ_0. These eigenvalues are all the branches of one or more multivalued functions analytic near β_0 with at worst algebraic singularities at β_0.

If A and B are self-adjoint, the perturbed eigenvalues of $A + \beta B$ are analytic at $\beta = 0$ even if A has degenerate eigenvalues. That the branch points allowed by the last theorem do not occur in this case is a theorem of Rellich. This theorem and its sister theorem on the analyticity of the eigenvectors in this case are the really deep results of finite-dimensional perturbation theory. The example at the beginning of this section shows that branch points can occur for *nonreal* β even in the "self-adjoint case," $T(\beta)^* = T(\bar{\beta})$.

Theorem XII.3 (Rellich's theorem) Suppose that $T(\beta)$ is a matrix-valued analytic function in a region R containing a section of the real axis, and that $T(\beta)$ is self-adjoint for β on the real axis. Let λ_0 be an eigenvalue of $T(\beta_0)$ of multiplicity m. If β_0 is *real*, there are $p \leq m$ distinct functions $\lambda_1(\beta)$, $\ldots$, $\lambda_p(\beta)$, *single-valued* and analytic in a neighborhood of β_0, which are *all* the eigenvalues.

Proof Consider one of the functions $\lambda_i(\beta)$ given in Theorem XII.2:

$$\lambda(\beta) = \lambda_0 + \sum_{j=1}^{\infty} \alpha_j (\beta - \beta_0)^{j/p}$$

The crucial fact that we shall use is that each branch of $\lambda(\beta)$ is an eigenvalue so that, in particular, *each branch is real for* β *real* and near β_0. Thus

$$\alpha_1 = \lim_{\beta \downarrow \beta_0} (\lambda(\beta) - \lambda_0) |\beta - \beta_0|^{-p^{-1}}$$

is real and

$$e^{i\pi/p}\alpha_1 = \lim_{\beta \uparrow \beta_0} (\lambda(\beta) - \lambda_0) |\beta - \beta_0|^{-p^{-1}}$$

is real. So, if $p \neq 1$, then $\alpha_1 = 0$. By induction, one shows that $\alpha_j = 0$ if j/p is not an integer. Therefore $\lambda(\beta)$ is actually analytic at $\beta = \beta_0$. ∎

We now want to consider the special case $H(\beta) = H_0 + \beta V$. Suppose that E_0 is a nondegenerate eigenvalue of H_0. From Theorem XII.1 we know that, for β small, $H_0 + \beta V$ has a unique eigenvalue $E(\beta)$ near E_0 and that $E(\beta)$ is analytic near $\beta = 0$. The coefficients of its Taylor series are called **Rayleigh–Schrödinger coefficients** and the Taylor series is called the **Rayleigh–Schrödinger series**. We can use the results described in the appendix to find formulas for the coefficients. The formulas are simpler when H_0 is self-adjoint, so we restrict ourselves to that case. $E(\beta)$ is the only eigenvalue of $H_0 + \beta V$ near E_0, so if $|E - E_0| < \varepsilon$, and ε is small, $E(\beta)$ is the only eigenvalue of $H_0 + \beta V$ in the circle $\{E \,|\, |E - E_0| < \varepsilon\}$. By the functional calculus,

$$P(\beta) = -\frac{1}{2\pi i} \oint_{|E - E_0| = \varepsilon} (H_0 + \beta V - E)^{-1} \, dE$$

is the projection onto the eigenvector with eigenvalue $E(\beta)$. We shall show in Theorem XII.9 that $(H_0 + \beta V - E)^{-1}$ is analytic in β near $\beta = 0$. Thus $P(\beta)$ is analytic in β at $\beta = 0$. In particular, if Ω_0 is the unperturbed eigenvector, then $P(\beta)\Omega_0 \neq 0$ for β small since $P(\beta)\Omega_0 \to \Omega_0$ as $\beta \to 0$. Since $P(\beta)\Omega_0$ is an unnormalized eigenvector for $H(\beta)$,

$$E(\beta) = \frac{(\Omega_0 \,,\, H(\beta)P(\beta)\Omega_0)}{(\Omega_0 \,,\, P(\beta)\Omega_0)} = E_0 + \beta \frac{(\Omega_0 \,,\, VP(\beta)\Omega_0)}{(\Omega_0 \,,\, P(\beta)\Omega_0)}$$

This formula is very important in the development of perturbation theory and plays a critical role in the discussions in Sections 2–4. For it says that to find the Taylor series for $E(\beta)$, we need only find the Taylor series for $P(\beta)$.

To do this, we need only find a Taylor series for $(H_0 + \beta V - E)^{-1}$ and integrate it. But the Taylor series for $(H_0 + \beta V - E)^{-1}$ is just a geometric series:

$$(H_0 + \beta V - E)^{-1} = (H_0 - E)^{-1} - \beta(H_0 - E)^{-1}V(H_0 - E)^{-1} + \cdots + (-1)^n\beta^n(H_0 - E)^{-1}[V(H_0 - E)^{-1}]^n + \cdots$$

Not only is this series simple, but there is a simple form for the error term when the series is truncated.

Thus, the Rayleigh–Schrödinger series for $E(\beta)$ is given by

$$E(\beta) = E_0 + \beta \frac{\sum_{n=0}^{\infty} a_n \beta^n}{\sum_{n=0}^{\infty} b_n \beta^n}$$

with

$$a_n = \frac{(-1)^{n+1}}{2\pi i} \oint_{|E-E_0|=\varepsilon} (\Omega_0 , [V(H_0 - E)^{-1}]^{n+1}\Omega_0)\, dE$$

$$b_n = \frac{(-1)^{n+1}}{2\pi i} \oint_{|E-E_0|=\varepsilon} (\Omega_0 , (H_0 - E)^{-1}[V(H_0 - E)^{-1}]^n\Omega_0)\, dE$$

Because of the contour integration and the division of power series, the formulas for the Rayleigh–Schrödinger coefficients are complicated. To illustrate this, let us compute $E(\beta)$ up to order β^4. Since H_0 is self-adjoint, we can choose a basis of eigenvectors, $\Omega_0, \ldots, \Omega_{n-1}$, with $H\Omega_i = E_i\Omega_i$. Let $V_{ij} = (\Omega_i, V\Omega_j)$. Then

$$b_0 = -\frac{1}{2\pi i} \oint_{|E-E_0|=\varepsilon} (\Omega_0 , (H_0 - E)^{-1}\Omega_0)\, dE$$

$$= -\frac{1}{2\pi i} \oint_{|E-E_0|=\varepsilon} (E_0 - E)^{-1}\, dE = 1$$

$$b_1 = \frac{1}{2\pi i} \oint_{|E-E_0|=\varepsilon} V_{00}(E_0 - E)^{-2}\, dE = 0$$

$$b_2 = -\frac{1}{2\pi i} \oint_{|E-E_0|=\varepsilon} (E_0 - E)^{-2} \sum_{i=0}^{n} (E_i - E)^{-1} V_{0i} V_{i0}\, dE$$

The $i = 0$ term in this last sum has a very different status from the $i \neq 0$ terms. For,

$$\frac{1}{2\pi i} \oint_{|E-E_0|=\varepsilon} (E_0 - E)^{-3}\, dE = 0$$

while

$$\frac{1}{2\pi i}\oint_{|E-E_0|=\varepsilon}(E_0-E)^{-2}(E_i-E)^{-1}\,dE=(E_i-E_0)^{-2}$$

Thus,

$$b_2=-\sum_{i\neq 0}(E_i-E_0)^{-2}V_{0i}V_{i0}$$

Similarly,

$$b_3=\sum_{i\neq 0\neq j}[(E_i-E_0)^{-1}(E_j-E_0)^{-2}+(E_i-E_0)^{-2}(E_j-E_0)^{-1}]V_{0i}V_{ij}V_{j0}$$
$$-2\sum_{i\neq 0}(E_i-E_0)^{-3}V_{0i}V_{i0}V_{00}$$

$$a_0=V_{00}$$

$$a_1=-\sum_{i\neq 0}(E_i-E_0)^{-1}V_{0i}V_{i0}$$

$$a_2=\sum_{i\neq 0\neq j}(E_i-E_0)^{-1}(E_j-E_0)^{-1}V_{0i}V_{ij}V_{j0}$$
$$-2\sum_{i\neq 0}(E_i-E_0)^{-2}V_{0i}V_{i0}V_{00}$$

$$a_3=-\sum_{\substack{i\neq 0\neq j\\ k\neq 0}}(E_i-E_0)^{-1}(E_j-E_0)^{-1}(E_k-E_0)^{-1}V_{0i}V_{ij}V_{jk}V_{k0}$$
$$+2\sum_{i\neq 0\neq j}[(E_i-E_0)^{-1}(E_j-E_0)^{-2}$$
$$+(E_j-E_0)^{-1}(E_i-E_0)^{-2}]V_{00}V_{0i}V_{ij}V_{j0}$$
$$+2\sum_{i\neq 0\neq j}(E_i-E_0)^{-2}(E_j-E_0)^{-1}V_{0i}V_{i0}V_{0j}V_{j0}$$
$$-3\sum_{i\neq 0}(E_i-E_0)^{-3}V_{0i}V_{i0}V_{00}^2$$

Thus, if we write $E(\beta)=E_0+\sum_{n=1}^{\infty}\alpha_n\beta^n$, we have computed:

$$\alpha_1=a_0=V_{00}$$

$$\alpha_2=a_1$$
$$=-\sum_{i\neq 0}(E_i-E_0)^{-1}V_{0i}V_{i0}$$

$$\alpha_3=a_2-b_2a_0$$
$$=\sum_{i\neq 0\neq j}(E_i-E_0)^{-1}(E_j-E_0)^{-1}V_{0i}V_{ij}V_{j0}-\sum_{i\neq 0}(E_i-E_0)^{-2}V_{0i}V_{i0}V_{00}$$

$$\alpha_4 = a_3 - b_3 a_0 - b_2 a_1$$
$$= -\sum_{\substack{i\neq 0\neq j\\ k\neq 0}} (E_i - E_0)^{-1}(E_j - E_0)^{-1}(E_k - E_0)^{-1} V_{0i} V_{ij} V_{jk} V_{k0}$$
$$+ \sum_{i\neq 0\neq j} [(E_i - E_0)^{-1}(E_j - E_0)^{-2}$$
$$+ (E_i - E_0)^{-2}(E_j - E_0)^{-1}] V_{00} V_{0i} V_{ij} V_{j0}$$
$$+ \sum_{i\neq 0\neq j} (E_i - E_0)^{-2}(E_j - E_0)^{-1} V_{0i} V_{i0} V_{0j} V_{j0}$$
$$- \sum_{i\neq 0} (E_i - E_0)^{-3} V_{0i} V_{i0} V_{00}^2$$

We can draw several conclusions from these elementary but tedious computations:

(i) The nth Rayleigh–Schrödinger coefficient α_n is considerably more complicated than the leading term

$$(-1)^{n+1} \sum_{i_1\neq 0,\, i_2\neq 0,\, \ldots,\, i_{n-1}\neq 0} \prod_{j=1}^{n-1} (E_{i_j} - E_0)^{-1} V_{0i_1} V_{i_1 i_2} \cdots V_{i_{n-1}0}$$

which one might guess from the familiar second-order term found in quantum-mechanics books.

(ii) The denominator in $(\Omega_0, VP(\beta)\Omega_0)/(\Omega_0, P(\beta)\Omega_0)$ does not add new complications to the Taylor series but actually provides cancellations with terms already present in the numerator.

(iii) Most importantly, the terms in the Taylor series are quite complicated, although they arise from a simple geometric series. This suggests that the simplest object to study is the resolvent: To deduce rigorous theorems about $E(\beta)$ in the infinite-dimensional case, we shall generally first prove results about the resolvent and then obtain information about the eigenvalues by formulas that give the eigenvalue as a ratio of contour integrals of matrix elements of the resolvent.

As a final result in finite-dimensional perturbation theory, we mention:

Theorem XII.4 Let Ω_0 be a nondegenerate eigenvector for T_0 with $T_0\Omega_0 = E_0\Omega_0$, and let $T(\beta)$ be a matrix-valued analytic function with $T(0) = T_0$. Then, for β small, there is a vector-valued analytic function $\Omega(\beta)$ that obeys $T(\beta)\Omega(\beta) = E(\beta)\Omega(\beta)$, where $E(\beta)$ is the eigenvalue of $T(\beta)$ near E_0. Moreover, if $T(\beta)$ is self-adjoint for β real, $\Omega(\beta)$ can be chosen so that $\|\Omega(\beta)\| = 1$ for β real.

Proof Take

$$\psi(\beta) = -\frac{1}{2\pi i}\oint_{|E-E_0|=\varepsilon}(T(\beta)-E)^{-1}\Omega_0\, dE \equiv P(\beta)\Omega_0$$

Then $\psi(\beta)$ is analytic and an eigenvector. Since $\psi(\beta)\to\Omega_0$ as $\beta\to 0$, $(\Omega_0, \psi(\beta))\neq 0$ for small β. Let $\Omega(\beta) = (\Omega_0, \psi(\beta))^{-1/2}\psi(\beta)$ Then $\Omega(\beta)$ is normalized when $T(\beta)$ is self-adjoint for β real since then $(\Omega_0, \psi(\beta)) = (\Omega_0, P(\beta)\Omega_0) = \|\psi(\beta)\|^2$. ∎

One can also construct analytic eigenvectors in the situation covered by Rellich's theorem; see Problems 16 and 17.

Appendix to XII.1 Algebraic and geometric multiplicity of eigenvalues of finite matrices

We first recall some elementary definitions about roots of algebraic equations:

Definition A root λ_0 of an algebraic equation $F(\lambda) = \lambda^n + a_1\lambda^{n-1} + \cdots a_n$ is called **nondegenerate** or **simple** if $F'(\lambda_0)\neq 0$. Equivalently λ_0 is simple if the decomposition $F(\lambda) = \prod_{i=1}^{n}(\lambda-\lambda_i)$ has $\lambda_i = \lambda_0$ for exactly one value of i. λ_0 is said to have **multiplicity** m if $F'(\lambda_0) = \cdots = F^{(m-1)}(\lambda_0) = 0$, $F^{(m)}(\lambda_0)\neq 0$ or equivalently if exactly m of the λ_i equal λ_0. An eigenvalue of a matrix is called **simple** or **nondegenerate** if it is a nondegenerate root of the secular equation. In general, the **algebraic multiplicity** of an eigenvalue is its multiplicity as a root of the secular equation.

The connection between algebraic multiplicity and geometric multiplicity is explained by the following series of remarks:

(i) Let $\mu(\lambda)$ be the algebraic multiplicity of λ. The fundamental theorem of algebra immediately implies that $\sum_{\lambda\in\mathbf{C}}\mu(\lambda) = n$ if T is an $n\times n$ matrix.

(ii) Let $m(\lambda) = \dim\{v \mid Tv = \lambda v\}$ be the **geometric multiplicity**. Then $m(\lambda)\leq\mu(\lambda)$.

(iii) If T is self-adjoint, $m(\lambda) = \mu(\lambda)$.

(iv) In general $\mu(\lambda) = \dim\{v\mid(T-\lambda)^k v = 0 \text{ for some } k\}$. This space is called the **generalized** or **geometric eigenspace** for λ.

The statements (ii) and (iv) become transparent once it is known that T can be put in Jordan normal form, i.e., there is a basis in which T has the block form

$$T = \left[\begin{array}{c|c|c|c} T_{\lambda_1} & 0 & 0 & 0 \\ \hline 0 & \ddots & 0 & 0 \\ \hline 0 & 0 & \ddots & 0 \\ \hline 0 & 0 & 0 & T_{\lambda_n} \end{array}\right]$$

$$T_{\lambda_i} = \begin{bmatrix} \lambda_i & x & 0 & & \cdots & 0 \\ 0 & \lambda_i & x & 0 & \cdots & 0 \\ 0 & 0 & \lambda_i & x & & 0 \\ & \cdots & & & & \\ & \cdots & & & & x \\ & \cdots & & & & \lambda_i \end{bmatrix}$$

where each $x = 0$ or 1. In this case, the generalized eigenspace $\{v | (T - \lambda_i)^k v = 0\}$ is spanned by the $\mu(\lambda_i)$ basis elements associated with the block T_{λ_i} and clearly $\mu(\lambda_i)$ is the number of times λ_i appears as a root of $\det(T - \lambda) = 0$.

From the fact that any matrix can be put in Jordan normal form, it is also easy to see (Problem 2) that if ε is chosen sufficiently small, then

$$P_{\lambda_i} = -\frac{1}{2\pi i} \oint_{|\lambda - \lambda_i| = \varepsilon} (T - \lambda)^{-1} \, d\lambda$$

is the projection onto the generalized eigenspace associated with λ_i and $P_{\lambda_i} P_{\lambda_j} = \delta_{ij} P_{\lambda_i}$. In fact, one of the ways of establishing properties (i)–(iv) is through the use of these P_{λ_i} (see Problems 3 and 4).

XII.2 Regular perturbation theory

We now turn to the main result of this chapter and prove that under very general circumstances the Rayleigh–Schrödinger series has a nonzero radius of convergence for perturbations of unbounded operators in infinite-dimensional Hilbert spaces. An example where such results are applicable is $H(\beta) = -\Delta + \beta V$ on $\mathbb{R}^3$ where $V \in L^2$ is real-valued and β is real and positive. We shall see in Section XIII.4 that $\sigma_{\text{ess}}(H(\beta)) = [0, \infty)$ and in Section

XIII.1 that $\inf \sigma(H(\beta)) \equiv E(\beta)$ is a monotonic decreasing function of β. If V is negative in some region of $\mathbb{R}^3$, $E(\beta)$ will be negative for β larger than some β_0 and thus, by the result on $\sigma_{\text{ess}}(H(\beta))$, an eigenvalue. It is reasonable to ask if this "ground state energy" $E(\beta)$ is analytic in β, at least in a neighborhood of the interval (β_0, ∞).

This section is divided into four parts: (1) A brief discussion of the discrete spectra of not necessarily self-adjoint operators. (2) A proof of the analyticity of discrete eigenvalues in the nondegenerate case for "analytic families of operators." This is the general theory of regular perturbations. This theory has many applications in quantum mechanics where eigenvalues are possible values of the energy. For this reason, we shall sometimes use the words **energy level** in place of eigenvalue. Another term we borrow from quantum mechanics is **coupling constant**, which we shall use for the variable β. (3) Two simple criteria (type (A) and type (B)) for $H_0 + \beta V$ to be an analytic family; these techniques enable one to apply the general theory to specific cases. (4) A brief discussion of degenerate perturbation theory.

We defined the discrete spectrum of a self-adjoint operator A in Section VII.3. For such operators, $\lambda \in \sigma_{\text{disc}}(A)$ means that λ is an isolated point of $\sigma(A)$ and $\dim P_{\{\lambda\}} < \infty$ where P_Ω is the projection-valued measure associated with A. In the case of a general operator, we obviously should keep the requirement that λ be an isolated point of $\sigma(A)$. To replace the spectral projection, we use the projection which we introduced in Section XII.1:

Theorem XII.5 Suppose that A is a closed operator and let λ be an isolated point of $\sigma(A)$. Explicitly, suppose that $\{\mu \,|\, |\mu - \lambda| < \varepsilon\} \cap \sigma(A) = \{\lambda\}$. Then,

(a) For any r with $0 < r < \varepsilon$,

$$P_\lambda = -\frac{1}{2\pi i} \oint_{|\mu-\lambda|=r} (A - \mu)^{-1}\, d\mu$$

exists and is independent of r.

(b) $P_\lambda^2 = P_\lambda$. Thus P_λ is a (*not necessarily orthogonal*) projection.

(c) If $G_\lambda = \text{Ran } P_\lambda$ and $F_\lambda = \text{Ker } P_\lambda$, then G_λ and F_λ are complementary (not necessarily orthogonal) closed subspaces; that is, $G_\lambda + F_\lambda = \mathscr{H}$ and $G_\lambda \cap F_\lambda = \{0\}$. Moreover, A leaves G_λ and F_λ invariant in the following precise sense: $G_\lambda \subset D(A)$, $AG_\lambda \subset G_\lambda$, $F_\lambda \cap D(A)$ is dense in F_λ, and $A[F_\lambda \cap D(A)] \subset F_\lambda$.

(d) If $\psi \in G_\lambda$ and G_λ is finite dimensional, then $(A - \lambda)^n \psi = 0$ for some n. If $B \equiv A \restriction F_\lambda$, then $\lambda \notin \sigma(B)$.

Proof (a) We already know that $(A-\mu)^{-1}$ is an analytic function on $\mathbb{C}\backslash\sigma(A) \equiv \rho(A)$. Thus the integral exists as a Banach-space-valued Riemann integral. That it is independent of r is a consequence of the Cauchy integral theorem.

(b) Let $r < R < \varepsilon$. Then, using the resolvent equation,

$$P_\lambda^2 = (2\pi i)^{-2} \oint_{|\mu-\lambda|=r} \oint_{|\nu-\lambda|=R} (A-\mu)^{-1}(A-\nu)^{-1}\, d\nu\, d\mu$$

$$= (2\pi i)^{-2} \oint_{|\mu-\lambda|=r} \oint_{|\nu-\lambda|=R} (\nu-\mu)^{-1}[(A-\nu)^{-1} - (A-\mu)^{-1}]\, d\mu\, d\nu$$

$$= (2\pi i)^{-2} \left[\oint_{|\nu-\lambda|=R} d\nu (A-\nu)^{-1} \oint_{|\mu-\lambda|=r} d\mu (\nu-\mu)^{-1} \right.$$

$$\left. - \oint_{|\mu-\lambda|=r} d\mu (A-\mu)^{-1} \oint_{|\nu-\lambda|=R} d\nu (\nu-\mu)^{-1} \right]$$

$$= (2\pi i)^{-2} \left[\oint_{|\nu-\lambda|=R} (A-\nu)^{-1} 0\, d\nu - \oint_{|\mu-\lambda|=r} (2\pi i)(A-\mu)^{-1}\, d\mu \right] = P_\lambda$$

(c) That $G_\lambda = \mathrm{Ker}(1-P_\lambda)$ and $F_\lambda = \mathrm{Ker}\, P_\lambda$ are closed complementary subspaces is elementary algebra (see Problem 6). Let $\psi = P_\lambda \psi \in G_\lambda$. Since P_λ is given by a Riemann integral, $\psi = \lim_{n\to\infty} \psi_n$ where

$$\psi_n = \sum_{i=1}^{n} c_i^{(n)} (A - \mu_i^{(n)})^{-1} \psi$$

and the $c_i^{(n)}$ and $\mu_i^{(n)}$ are chosen so that the sums converge to $-(2\pi i)^{-1} \oint (A-\mu)^{-1}\psi\, d\mu$. A simple computation using the formula $A(A-\mu)^{-1} = 1 + \mu(A-\mu)^{-1}$ proves that $\psi_n \to \psi$ and that $\{A\psi_n\}$ is Cauchy. Since A is closed, we conclude that $\psi \in D(A)$ and the above approximation procedure proves that $A\psi = AP_\lambda\psi = P_\lambda(A\psi)$. Thus $A\psi \in G_\lambda$. The statements about $D(A)$ and F_λ are left to the reader.

(d) Suppose that $A\psi = \nu\psi$. Then

$$P_\lambda \psi = (-2\pi i)^{-1} \oint_{|\mu-\lambda|=r} (\nu-\mu)^{-1}\psi\, d\mu = \begin{cases} \psi & \text{if } \nu = \lambda \\ 0 & \text{if } \nu \neq \lambda \end{cases}$$

It follows that the only eigenvalue of $A \restriction G_\lambda$ is λ. If G_λ is finite dimensional, the Jordan normal form of $C \equiv A \restriction G_\lambda$ has only λ along the diagonal and some 1's above the diagonal. Thus $(C-\lambda)^{(\dim G_\lambda)} = 0$, i.e., $(A-\lambda)^n\psi = 0$ for all $\psi \in G_\lambda$.

Finally, let

$$R_\lambda = (-2\pi i)^{-1} \oint_{|\mu-\lambda|=r} (\lambda-\mu)^{-1}(A-\mu)^{-1}\, d\mu$$

By doing computations similar to those in (b), one finds that $R_\lambda P_\lambda = P_\lambda R_\lambda$ and that $(A-\lambda)R_\lambda = R_\lambda(A-\lambda) = 1 - P_\lambda$. $R_\lambda(A-\lambda) = 1-P_\lambda$ indicates an operator equality applied to vectors in $D(A)$. Thus R_λ takes F_λ into itself and $(B-\lambda)R_\lambda = R_\lambda(B-\lambda) = I \restriction F_\lambda$. ∎

We are now in a position to define discrete spectrum:

Definition A point $\lambda \in \sigma(A)$ is called **discrete** if λ is isolated and P_λ (given by Theorem XII.5) is finite dimensional; if P_λ is one dimensional, we say λ is a **nondegenerate** eigenvalue.

The reader should check that this definition of discrete spectrum agrees with the definition given in Chapters VII and VIII when A is self-adjoint. Note that if λ is a nondegenerate eigenvalue, any $\psi \in \text{Ran } P_\lambda$ obeys $A\psi = \lambda\psi$. To complete our discussion of the discrete spectrum, we prove a converse to Theorem XII.5.

Theorem XII.6 Let A be an operator with $\{\mu \,|\, |\mu-\lambda| = r\} \subset \rho(A)$. Then $P = (-2\pi i)^{-1} \oint_{|\mu-\lambda|=r}(A-\mu)^{-1}\, d\mu$ is a projection. If P has dimension $n < \infty$, then A has at most n points of its spectrum in $\{\mu \,|\, |\mu-\lambda| < r\}$ and each is discrete. If $n = 1$, there is exactly one spectral point in $\{\mu \,|\, |\mu-\lambda| < r\}$ and it is nondegenerate.

Proof The proof of Theorem XII.5b carries through without change to prove that P is a projection and the proof of (c) implies that $G = \text{Ran } P$ and $F = \text{Ker } P$ are closed complementary invariant subspaces. Let $A_1 = A \restriction G$ and $A_2 = A \restriction F$. As in the proof of Theorem XII.5d, $\nu \notin \sigma(A_2)$ if $|\nu - \lambda| < r$. Thus $(A-\nu)^{-1}$ exists for such ν if and only if $(A_1 - \nu)^{-1}$ exists. If G is finite dimensional, A_1 has eigenvalues $\nu_1, \ldots, \nu_k$ $(k \le n)$, so $\sigma(A) \cap \{\nu \,|\, |\nu-\lambda| < r\}$ is a finite set. To see that each spectral point in the circle is discrete, we note that if P_ν is the spectral projection of Theorem XII.5 and if ν is in the circle, then $P_\nu P = P P_\nu = P_\nu$. Thus Ran $P_\nu \subset$ Ran P, which completes the proof. ∎

Having completed our brief discussion of discrete spectra, we can get down to the real object of study:

Definition A (possibly unbounded) operator-valued function $T(\beta)$ on a complex domain R is called an **analytic family** or an **analytic family in the sense of Kato** if and only if:

(i) For each $\beta \in R$, $T(\beta)$ is closed and has a nonempty resolvent set.
(ii) For every $\beta_0 \in R$, there is a $\lambda_0 \in \rho(T(\beta_0))$ so that $\lambda_0 \in \rho(T(\beta))$ for β near β_0 and $(T(\beta) - \lambda_0)^{-1}$ is an analytic operator-valued function of β near β_0.

If $T(\beta)$ is a family of bounded operators, this definition is equivalent to the definition of bounded operator-valued analytic function (Problem 8). The number λ_0 in the above definition does not play a special role:

Theorem XII.7 Let $T(\beta)$ be an analytic family on a domain R. Then

$$\Gamma = \{\langle \beta, \lambda \rangle \mid \beta \in R, \lambda \in \rho(T(\beta))\}$$

is open and the function $(T(\beta) - \lambda)^{-1}$ defined on Γ is an analytic function of two variables.

Proof Let $\langle \beta_0, \lambda_1 \rangle \in \Gamma$ and suppose that $(T(\beta) - \lambda_0)^{-1}$ exists and is analytic in β for β near β_0. By the first resolvent identity, $1 - (\lambda_1 - \lambda_0) \times (T(\beta_0) - \lambda_0)^{-1}$ has an inverse equal to $(T(\beta_0) - \lambda_0)(T(\beta_0) - \lambda_1)^{-1}$. Since the set of invertible operators in $\mathscr{L}(\mathscr{H})$ is open, $[1 - (\lambda - \lambda_0)(T(\beta) - \lambda_0)^{-1}]$ is invertible if λ is near λ_1 and β is near β_0. For such $\langle \beta, \lambda \rangle$, $T(\beta) - \lambda$ has an inverse equal to

$$(T(\beta) - \lambda_0)^{-1}[1 - (\lambda - \lambda_0)(T(\beta) - \lambda_0)^{-1}]^{-1}$$

so $\langle \beta, \lambda \rangle \in \Gamma$. Thus Γ is open. To prove the analyticity of $(T(\beta) - \lambda)^{-1}$, we note that $1 - (\lambda - \lambda_0)(T(\beta) - \lambda_0)^{-1}$ is analytic for λ near λ_0 and β near β_0 with values in the invertible operators. By a general theorem (Problem 9), it follows that $(1 - (\lambda - \lambda_0)(T(\beta) - \lambda_0)^{-1})^{-1}$ and therefore $(T(\beta) - \lambda)^{-1}$ is analytic. ∎

Only a simple technical lemma remains to complete the machinery for an effortless proof of the Kato–Rellich theorem:

Lemma If P and Q are two (not necessarily orthogonal) projections and $\dim(\text{Ran } P) \neq \dim(\text{Ran } Q)$, then $\|P - Q\| \geq 1$. In particular, if $P(x)$ is a continuous projection-valued function of x on a connected topological space, then $\dim(\text{Ran } P(x))$ is a constant.

Proof Without loss of generality suppose $\dim(\text{Ran } P) < \dim(\text{Ran } Q)$. Let $F = \text{Ker } P$ and let $E = \text{Ran } Q$. Then $\dim(F^{\perp}) = \dim(\text{Ran } P) < \dim E$. As a result, $F \cap E \neq \{0\}$ (see Problem 4 of Chapter X). Let $\psi \neq 0$, $\psi \in F \cap E$. Then $P\psi = 0$, $Q\psi = \psi$, so $\|(P - Q)\psi\| = \|\psi\|$. This implies that $\|P - Q\| \geq 1$. The final statement follows from an elementary connectedness argument. ∎

Theorem XII.8 (Kato–Rellich theorem) Let $T(\beta)$ be an analytic family in the sense of Kato. Let E_0 be a nondegenerate discrete eigenvalue of $T(\beta_0)$. Then, for β near β_0, there is exactly one point $E(\beta)$ of $\sigma(T(\beta))$ near E_0 and this point is isolated and nondegenerate. $E(\beta)$ is an analytic function of β for β near β_0, and there is an analytic eigenvector $\Omega(\beta)$ for β near β_0. If $T(\beta)$ is self-adjoint for $\beta - \beta_0$ real, then $\Omega(\beta)$ can be chosen to be normalized for $\beta - \beta_0$ real.

Proof Pick ε so that the only point of $\sigma(T(\beta_0))$ within $\{E \,|\, |E - E_0| \leq \varepsilon\}$ is E_0. Since the circle $\{E \,|\, |E - E_0| = \varepsilon\}$ is compact and the set Γ of the last theorem is open, we can find δ so that $E \notin \sigma(T(\beta))$ if $|E - E_0| = \varepsilon$ and $|\beta - \beta_0| \leq \delta$. Let $N = \{\beta \,|\, |\beta - \beta_0| \leq \delta\}$. Then

$$P(\beta) = -(2\pi i)^{-1} \oint_{|E - E_0| = \varepsilon} (T(\beta) - E)^{-1}\, dE$$

exists and is analytic for $\beta \in N$. The nondegeneracy of E_0 as an eigenvalue of $T(\beta_0)$ implies that $P(\beta_0)$ is one dimensional. The last lemma then implies $P(\beta)$ is one dimensional for all $\beta \in N$. Thus, by Theorem XII.6, there is exactly one eigenvalue $E(\beta)$ of $T(\beta)$ with $|E(\beta) - E_0| < \varepsilon$ when $\beta \in N$ and this eigenvalue is nondegenerate. The analyticity of $E(\beta)$ follows from the formula

$$(E(\beta) - E_0 - \varepsilon)^{-1} = \frac{(\Omega_0\,,\, (T(\beta) - E_0 - \varepsilon)^{-1} P(\beta)\Omega_0)}{(\Omega_0\,,\, P(\beta)\Omega_0)}$$

We obtain an analytic eigenvector by choosing $\Omega(\beta) = P(\beta)\Omega_0$ or

$$\Omega(\beta) = (\Omega_0\,,\, P(\beta)\Omega_0)^{-1/2} P(\beta)\Omega_0$$

in the real case, where Ω_0 is the unperturbed eigenvector. ∎

We thus see how easy it is to prove that energy levels are analytic in the coupling constant *if* we know that $T(\beta)$ is an analytic family. This would not be very useful if we did not have convenient criteria for $T(\beta)$ to be analytic. Fortunately, there are two simple ones reflecting the usual operator/form

dualism. We shall discuss the operator criterion in detail and the form criterion briefly.

Definition Let R be a connected domain in the complex plane and let $T(\beta)$, a closed operator with nonempty resolvent set, be given for each $\beta \in R$. We say that $T(\beta)$ is an **analytic family of type (A)** if and only if

(i) The operator domain of $T(\beta)$ is some set D independent of β.
(ii) For each $\psi \in D$, $T(\beta)\psi$ is a vector-valued analytic function of β.

Of course, every family of type (A) is an analytic family in the sense of Kato. We leave the general case of this theorem to the problems and consider only the linear case $T(\beta) = H_0 + \beta V$. We first prove a lemma that is of interest in itself since it is a convenient criterion for a family to be type (A).

Lemma Let H_0 be a closed operator with nonempty resolvent set. Define $H_0 + \beta V$ on $D(H_0) \cap D(V)$. Then $H_0 + \beta V$ is an analytic family of type (A) near $\beta = 0$ if and only if:

(a) $D(V) \supset D(H_0)$.
(b) For some a and b and for all $\psi \in D(H_0)$,

$$\|V\psi\| \leq a\|H_0\psi\| + b\|\psi\|$$

That is, $H_0 + \beta V$ is type (A) if and only if V is H_0-bounded in the sense of Section X.2.

Proof Suppose first that $H_0 + \beta V$ is an analytic family of type (A). Then $D(H_0) = D(H_0 + \beta V) = D(H_0) \cap D(V)$ so (a) holds. Since H_0 is closed, $D(H_0)$ with the norm $|||\psi||| = \|H_0\psi\| + \|\psi\|$ is a Banach space $\hat{D}$. Fix β small and positive so that β and $-\beta$ are both in the domain of analyticity. $H_0 + \beta V: \hat{D} \to \mathscr{H}$ is everywhere defined and has a closed graph in $\hat{D} \times \mathscr{H}$ since the graph is closed in $\mathscr{H} \times \mathscr{H}$ with a weaker topology. Thus, by the closed graph theorem,

$$\|(H_0 + \beta V)\psi\| \leq a_1|||\psi|||$$

and

$$\|(H_0 - \beta V)\psi\| \leq a_2|||\psi|||$$

Thus,

$$\begin{aligned}\|V\psi\| &\leq (2\beta)^{-1}[\|(H_0 + \beta V)\psi\| + \|(H_0 - \beta V)\psi\|] \\ &\leq (2\beta)^{-1}(a_1 + a_2)|||\psi|||\end{aligned}$$

so that condition (b) holds.

Conversely, let (a) and (b) hold. Then, for $\psi \in D(H_0)$,

$$\begin{aligned}\|H_0\psi\| &\leq \|(H_0 + \beta V)\psi\| + |\beta|\,\|V\psi\| \\ &\leq \|(H_0 + \beta V)\psi\| + |\beta|a\|H_0\psi\| + |\beta|b\|\psi\|\end{aligned}$$

Thus, if $|\beta| < a^{-1}$, we have

$$\|H_0\psi\| \leq (1 - |\beta|a)^{-1}\|(H_0 + \beta V)\psi\| + (1 - |\beta|a)^{-1}b|\beta|\,\|\psi\|$$

Therefore, $H_0 + \beta V$ is closed on $D(H_0)$ for if $\psi_n \to \psi$ in $\mathscr{H}$ with $\psi_n \in D(H_0)$ and $(H_0 + \beta V)\psi_n$ is Cauchy, then $H_0\psi_n$ is Cauchy by the above inequality and thus $\psi \in D(H_0)$. That $(H_0 + \beta V)\psi$ is analytic for $\psi \in D(H_0)$ is obvious. ∎

It is a corollary of the above proof that if V is infinitesimally small with respect to H_0, then $H_0 + \beta V$ is an *entire* family of type (A).

Example 1 Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$. More generally, let $V = \sum V_{ij}$ with $V_{ij} \in L^2 + L^\infty$ and $H_0 = -\Delta$ on $\mathbb{R}^{3n}$. Then $H_0 + \beta V$ is an entire analytic family of type (A).

Example 2 It can be shown that if $V << H_0$ and $W << H_0$, then $W << H_0 + V$ (Problem 11). Thus, letting $H_0 = -\Delta_1 - \Delta_2 - 2/r_1 - 2/r_2$ on $L^2(\mathbb{R}^6)$ and $V = |r_1 - r_2|^{-1}$, we see $H_0 + \beta V$ is an analytic family of type (A). In the approximation of infinite nuclear mass, $H + V$ is the helium atom Hamiltonian (see Section XI.5 for the kinematics).

Theorem XII.9 Let $H_0 + \beta V$ be an analytic family of type (A) in a region R. Then $H_0 + \beta V$ is an analytic family in the sense of Kato. In particular, if $0 \in R$ and if E_0 is an isolated nondegenerate eigenvalue of H_0, then there is a unique point $E(\beta)$ of $\sigma(H_0 + \beta V)$ near E_0 when $|\beta|$ is small which is an isolated nondegenerate eigenvalue. Moreover, $E(\beta)$ is analytic near $\beta = 0$.

Proof Since analyticity is a local property, we suppose that $0 \in R$ and prove analyticity in the sense of Kato near $\beta = 0$. Choose $\lambda \notin \sigma(H_0)$. Then $(H_0 - \lambda)^{-1}$ and $H_0(H_0 - \lambda)^{-1} = 1 + \lambda(H_0 - \lambda)^{-1}$ are bounded. Thus, for any $\varphi \in \mathscr{H}$,

$$\begin{aligned}\|V(H_0 - \lambda)^{-1}\varphi\| &\leq a\|H_0(H_0 - \lambda)^{-1}\varphi\| + b\|(H_0 - \lambda)^{-1}\varphi\| \\ &\leq (a\|H_0(H_0 - \lambda)^{-1}\| + b\|(H_0 - \lambda)^{-1}\|)\|\varphi\|\end{aligned}$$

Thus $V(H_0 - \lambda)^{-1}$ is bounded; so for β small, $[1 + \beta V(H_0 - \lambda)^{-1}]^{-1}$ exists and is analytic in β (being given by a geometric series). Direct computation (Problem 12) shows that $(H_0 - \lambda)^{-1}[1 + \beta V(H_0 - \lambda)^{-1}]^{-1}$ is an inverse for $(H_0 + \beta V - \lambda)$, so for β small, $\lambda \notin \sigma(H_0 + \beta V)$ and $(H_0 + \beta V - \lambda)^{-1}$ is analytic in β. This proves that $H_0 + \beta V$ is an analytic family in the sense of Kato near $\beta = 0$. By writing $H_0 + \beta V = (H_0 + \beta_0 V) + (\beta - \beta_0)V$, we prove analyticity at $\beta = \beta_0$. ∎

Example 1, revisited By Theorem X.15 and Theorem XII.9, it follows that $E_0(\beta)$, the lowest eigenvalue of $-\Delta + \beta V$ is an analytic function of β in a neighborhood of (β_0, ∞) where $\beta_0 = \inf\{\beta > 0 \,|\, E_0(\beta) < 0\}$. In applying Theorem XII.9, we are assuming the nondegeneracy of the ground state which we shall prove in Section XIII.12.

Example 2, revisited $h \equiv -\Delta_1 - 2/r_1$ is an operator with an exactly solvable eigenvalue problem. Its lowest eigenvalue is $E = -1$. H_0 is of the form $h \otimes 1 + 1 \otimes h$ on $L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3) = L^2(\mathbb{R}^6)$, so its ground state energy is -2. For $|\beta|$ small, the ground state energy $E(\beta)$ is analytic with the Taylor coefficients at $\beta = 0$ given by the Rayleigh–Schrödinger formula discussed in Section 1.

Physically, one is interested in the ground state energy $E(1)$ of the helium atom. The question immediately arises as to whether the Taylor series for $E(\beta)$ about $\beta = 0$ has a radius of convergence bigger than 1. In Theorem XII.11 below, we shall obtain explicit lower bounds on the radius of convergence of the Rayleigh–Schrödinger series, but our bounds will be crude and we shall not be able to use them directly to prove that $\beta = 1$ is within the circle of convergence. By hard work one might be able to show $\beta = 1$ is actually in the circle of convergence (we expect it is true), but the question is really academic! For when $\beta = 1$, even if the series is convergent, a large number of terms of the Taylor series are necessary to approximate $E(1)$ well, and the higher order Rayleigh–Schrödinger coefficients are hard to compute. For example, the first-order approximate value $(\Omega_0, V\Omega_0)$ for $E(1) - E(0)$ disagrees with experiment by about 15%. It turns out that other methods, which we shall discuss in Section XIII.2, can be used to obtain an accuracy of better than 1% with experiment (and if various relativistic corrections are taken into account, of one part in 10^6). However, if β is small, perturbation theory is more accurate. It turns out that the ground state energy of Li^+ is directly related to $E(\frac{4}{9})$ and it is given by the first-order approximant to within 5%. $E(\frac{1}{4})$, which is related to the ground state energy of Be^{++}, is given within 2%.

Example 3 (hyperfine structure in hydrogen) Perturbation theory is connected with one of the more spectacular agreements between theory and experiment in quantum physics. In the usual model for the hydrogen atom there is one energy level near -13 eV, the ground state energy. The physical atom has two levels; this splitting is due to interactions between the magnetic moments of the electron and proton. It is the transition between these levels that radio astronomers observe when looking for intergalactic gas clouds, and it is this transition that is the dominant one in a hydrogen maser. For the latter reason, the energy difference is very well measured; in fact, in units with $\hbar = 1$, so that ΔE has units of hertz (Hz) $\equiv$ cycles per second,

$$\Delta E(1s_{1/2}) = 1{,}420{,}405{,}751.800 \quad \text{Hz}$$

There is an old theory of the magnetic interaction due to Fermi and Segrè which is suggested by classical models of interacting magnets. The Fermi–Segrè potential has a coupling constant β made up of fundamental constants (magnetic moments of the electron and proton, the electric charge), a spin–spin interaction and multiplication by $\rho(r)$, the effective charge distribution of the proton. In practice $\rho(r)$ is approximated by a δ function, which means that it is technically outside the mathematical theory we have discussed, but a peaked smooth function $\rho(r)$ is within our theory, and leads to approximately the same lowest order contributions to perturbation theory.

In comparing theory and experiment an interesting problem arises. The physical constants needed to compute β are known to only about one part in 10^5 or 10^6 and $\Delta E(1s_{1/2}) = \beta a_1 + \beta^2 a_2 + \cdots$, where $\beta \simeq 10^{-4}$ and a_1, a_2, measured in units of the ground state energy of hydrogen, are about 1. For a truly accurate comparison with experiment, one also looks at the hyperfine splitting in the first excited state $\Delta E(2s_{1/2}) = \beta b_1 + \beta^2 b_2$. If we look at the ratio $\Delta E(2s_{1/2})/\Delta E(1s_{1/2})$, then since β is already approximately 10^{-4}, an error of β in its sixth place only affects $(a_1 + \beta a_2)/(b_1 + \beta b_2)$ in its tenth place! Experimentally:

$$\frac{\Delta E(2s_{1/2})}{\Delta E(1s_{1/2})} = \frac{1}{8}(1.000034495)$$

The Fermi–Segrè theory (with relativistic corrections) and lower order perturbation theory predicts

$$\frac{\Delta E(2s_{1/2})}{\Delta E(1s_{1/2})} = \frac{1}{8}(1.00003445)$$

Better agreement than this would actually be embarrassing since the above calculations ignore the finite size of the nucleus, corrections due to strong interactions, etc.

Let us return to general criteria for a linear function $H_0 + \beta V$ to be an analytic family in the sense of Kato. There is a form notion analogous to the operator notion of family of type (A). An **analytic family of type (b)** is a family of closed, strictly m-sectorial forms, $q(\beta)$, one for each β in a region R of the complex plane, so that:

(i) The form domain of $q(\beta)$ is some subspace F independent of β.
(ii) $(\psi, q(\beta)\psi)$ is an analytic function in R for each $\psi \in F$.

If $q(\beta)$ is an analytic family of type (b), then, for each $\beta \in R$, there is associated a unique closed operator $T(\beta)$ by Theorem VIII.16. $T(\beta)$ is called an **analytic family of type (B)**. As in the type (A) case, any analytic family of type (B) is an analytic family in the sense of Kato, and $H_0 + \beta V$ defined as a form on $Q(H_0) \cap Q(V)$ is an analytic family of type (B) near $\beta = 0$ if and only if V is H_0 form bounded.

Type (B) methods can be used to extend the results discussed under Example 1 above to potentials in the Rollnik class $R + L^\infty$. Type (B) techniques imply strong analyticity properties for $H_0 + \beta V$ if H_0 and V are positive:

Theorem XII.10 Let H_0 be positive and self-adjoint and let V be self-adjoint. Let $V_+ = \frac{1}{2}(V + |V|)$; $V_- = \frac{1}{2}(|V| - V)$. Suppose that:

(i) $Q(V_+) \cap Q(H_0)$ is dense.
(ii) V_- is H_0 form bounded with relative bound zero.

Then $H_0 + \beta V$ is an analytic family of type (B) in the cut plane $\{\beta \,|\, \beta \notin (-\infty, 0]\}$.

A reference for the proof of this theorem can be found in the Notes.

Example 4 From our discussion in Section XIII.12, it will follow that the ground state of $-d^2/dx^2 + x^2 + \beta x^4$ is nondegenerate if $\beta > 0$. Thus, Theorem XII.10 says that its ground state energy $E(\beta)$ is analytic in a neighborhood of the positive real axis.

There are examples of analytic families that are neither type (A) nor type (B). For example, let $T(\beta)$ be an analytic family of type (A) and let C be any bounded self-adjoint operator. Then $U(\beta) = \exp(i\beta C)$ is an entire analytic function. It is not hard to see that $\tilde{T}(\beta) = U(\beta)T(\beta)U(\beta)^{-1}$, defined on $U(\beta)D$, is an analytic family. However, C and T can be chosen so that neither $D(T(\beta))$ nor $Q(T(\beta))$ is constant.

We would like to make a few remarks, some of which are warnings about pitfalls. First, we note that as in Section 1 one has explicit formulas for the coefficients of the Taylor series for $E(\beta)$ given as contour integrals of resolvents. If H_0 has purely discrete spectrum, we can do the integrals explicitly and obtain formulas identical to those of the preceding section. If H_0 is self-adjoint, we can still do these contour integrals, obtaining spectral integrals in place of sums; for example, if E_0 is an isolated nondegenerate eigenvalue of H_0 so that $\operatorname{dist}(E_0, \sigma(H_0)\backslash E_0) > \varepsilon$, then

$$\alpha_2 = -\int_{|\lambda - E_0| > \varepsilon} (\lambda - E_0)^{-1}\, d(V\Omega_0, P_\lambda V\Omega_0)$$

Secondly, we warn the reader that it may happen that the power series for $E(\beta)$ has a circle of convergence larger than the circle in which $H(\beta)$ has $E(\beta)$ as an eigenvalue.

Example 5 Let $H_0 = -\Delta - 1/r$ and $V = 1/r$. Then, the eigenvalues of $H_0 + \beta V$ for β small are $-\frac{1}{4}n^{-2}(1-\beta)^2$, $n = 1, 2, \ldots$. In particular, the ground state energy $(n = 1)$ $E_0(\beta) = -\frac{1}{4} + \frac{1}{2}\beta - \frac{1}{4}\beta^2$ is given by a function with an analytic continuation to the entire complex plane. But for $\beta > 1$, H_0 has no eigenvalues at all!

Thus, one vestige of the finite-dimensional theory is not present: In general, the analytic continuation of an eigenvalue need not be an eigenvalue. However, in one important special case it can be proven that the analytic continuation of an eigenvalue is an eigenvalue (see Problem 13).

Finally, we note that one can obtain explicit lower bounds on the radius of convergence of the Taylor series:

Theorem XII.11 Suppose that $\|V\varphi\| \leq a\|H_0\varphi\| + b\|\varphi\|$. Let H_0 be self-adjoint with an unperturbed isolated, nondegenerate eigenvalue E_0, and let $\varepsilon = \frac{1}{2}\operatorname{dist}(E_0, \sigma(H_0)\backslash\{E_0\})$. Define

$$r(a, b, E_0, \varepsilon) = [a + \varepsilon^{-1}[b + a(|E_0| + \varepsilon)]]^{-1}$$

Then the eigenvalue $E(\beta)$ of $H_0 + \beta V$ near E_0 is analytic in the circle of radius $r(a, b, E_0, \varepsilon)$.

The reader is asked to provide a proof in Problem 14.

* * *

As a final subject in regular perturbation theory, we shall discuss the case where E_0 is an isolated degenerate eigenvalue of finite multiplicity of $T(\beta_0)$. Because of our experience with the finite-dimensional case, we shall suppose that $T(\beta)$ is self-adjoint for β real. If $T(\beta)$ is a Kato family, we have no trouble in proving that $P(\beta) = (-2\pi i)^{-1} \oint (T(\beta) - E)^{-1}\, dE$ is analytic in β for β near β_0. We are thus faced with finding the eigenvalues of $H(\beta)$ restricted to the *variable* finite-dimensional subspace Ran $P(\beta)$. To reduce this to a truly finite-dimensional problem, we need the following technical result of Kato, which has several other applications (see Problems 15 and 17).

Theorem XII.12 Let R be a connected, simply connected region of the complex plane containing 0. Let $P(\beta)$ be a projection-valued analytic function in R. Then, there is an analytic family $U(\beta)$ of invertible operators with

$$U(\beta)P(0)U(\beta)^{-1} = P(\beta)$$

Moreover, if $P(\beta)$ is self-adjoint for β real and in R, then we can choose $U(\beta)$ unitary for β real.

We defer the proof to the conclusion of this section.

Theorem XII.13 Let $T(\beta)$ be an analytic family in the sense of Kato for β near 0 that is self-adjoint for β real. Let E_0 be a discrete eigenvalue of multiplicity m. Then, there are m not necessarily distinct single-valued functions, analytic near $\beta = 0$, $E^{(1)}(\beta), \ldots, E^{(m)}(\beta)$, with $E^{(k)}(0) = E_0$, so that $E^{(1)}(\beta), \ldots, E^{(m)}(\beta)$ are eigenvalues of $T(\beta)$ for β near 0 (with a repeated entry in $E^{(1)}, \ldots, E^{(m)}$ indicating a degenerate eigenvalue). Further, these are the only eigenvalues near E_0.

Proof Since E_0 is an isolated point of $\sigma(T(0))$, and $T(\beta)$ is an analytic family, $P(\beta) = (-2\pi i)^{-1} \oint (T(\beta) - E)^{-1}\, dE$ exists and is analytic for β small. By the proof of Theorem XII.6,

$$\sigma(T(\beta) \restriction \text{Ran } P(\beta)) = \sigma(T(\beta)) \cap \{E \,|\, |E - E_0| < \varepsilon\}$$

From Theorem XII.12 we know that there exists a family $U(\beta)$, analytic near $\beta = 0$, unitary for β real, so that $U(\beta)P(0)U(\beta)^{-1} = P(\beta)$. Let $\tilde{T}(\beta) = U(\beta)^{-1}T(\beta)U(\beta)$. Then Ran $P(0)$ is an invariant subspace for all the $\tilde{T}(\beta)$. Thus $S(\beta) \equiv \tilde{T}(\beta) \restriction \text{Ran } P(0)$ is a finite-dimensional analytic family, self-adjoint for β real. The theorem now follows from Rellich's theorem (Theorem XII.3). ∎

Since we have reduced the infinite-dimensional problem to a finite-dimensional one, the existence of analytic eigenvectors in the finite-dimensional case implies their existence in the infinite-dimensional case.

Example 1, revisited If $H_0 + \beta_0 V$ has n eigenvalues in $(-\infty, 0)$, then $H_0 + \beta V$ has at least n eigenvalues for $|\beta - \beta_0|$ small, and the ones near those of $H_0 + \beta_0 V$ are analytic in β near β_0.

Finally, we shall prove Theorem XII.12. The idea of the proof comes from differentiating $U(\beta)P(0)U(\beta)^{-1} = P(\beta)$, finding $P'(\beta) = [U'(\beta)U(\beta)^{-1}, P(\beta)]$ where $[A, B] = AB - BA$. Thus, one seeks an operator $Q(\beta)$ that satisfies $P'(\beta) = [Q(\beta), P(\beta)]$ and then solves the differential equation $U'(\beta) = Q(\beta)U(\beta)$.

Lemma Let R be a connected, simply connected subset of $\mathbb{C}$ with $0 \in R$ and let $A(\beta)$ be an analytic function on R with values in the bounded operators on some Banach space X. Then for any $x_0 \in X$, there is a unique function $f(\beta)$, analytic in R, with values in X obeying

$$\frac{d}{d\beta} f(\beta) = A(\beta) f(\beta), \qquad f(0) = x_0 \tag{2}$$

Proof By standard methods of analytic continuation, it is enough to suppose that R is a circle of radius r_0 and to show that there is an analytic solution in the circle of radius $r_0 - 2\varepsilon$ for any ε. We first note that uniqueness follows from (2): By supposing $f(\beta) = \sum_{n=0}^{\infty} f_n \beta^n$ and knowing $A(\beta) = \sum_{n=0}^{\infty} A_n \beta^n$, one finds that

$$f_0 = x_0 \tag{3a}$$

$$f_n = n^{-1} \left[\sum_{k=0}^{n-1} A_k \, f_{n-1-k} \right] \tag{3b}$$

We now show that if the f_n are defined by (3), then $\sum_{n=0}^{\infty} f_n \beta^n$ converges if $|\beta| < r_0 - 2\varepsilon$. Let $M = \max\{1 + \|A(\beta)\| \mid |\beta| \leq r_0 - \varepsilon\}$. By the Cauchy integral formula, $\|A_n\| < M(r_0 - \varepsilon)^{-n}$. A simple inductive argument using (3) shows that $\|f_n\| < (M(r_0 - \varepsilon)^{-1})^n \|x_0\|$. It follows that $f(\beta)$ is analytic in a circle of radius $(r_0 - \varepsilon)/M$. By repeating this argument at points β with $|\beta|$ near $(r_0 - \varepsilon)/M$, we can prove that f is analytic in a circle of radius $(r_0 - \varepsilon)M^{-1} + M^{-1}(r_0 - \varepsilon)(1 - M^{-1})$. See Figure XII.1. After a finite number of repetitions we get analyticity in a circle of radius $r_0 - 2\varepsilon$. ∎

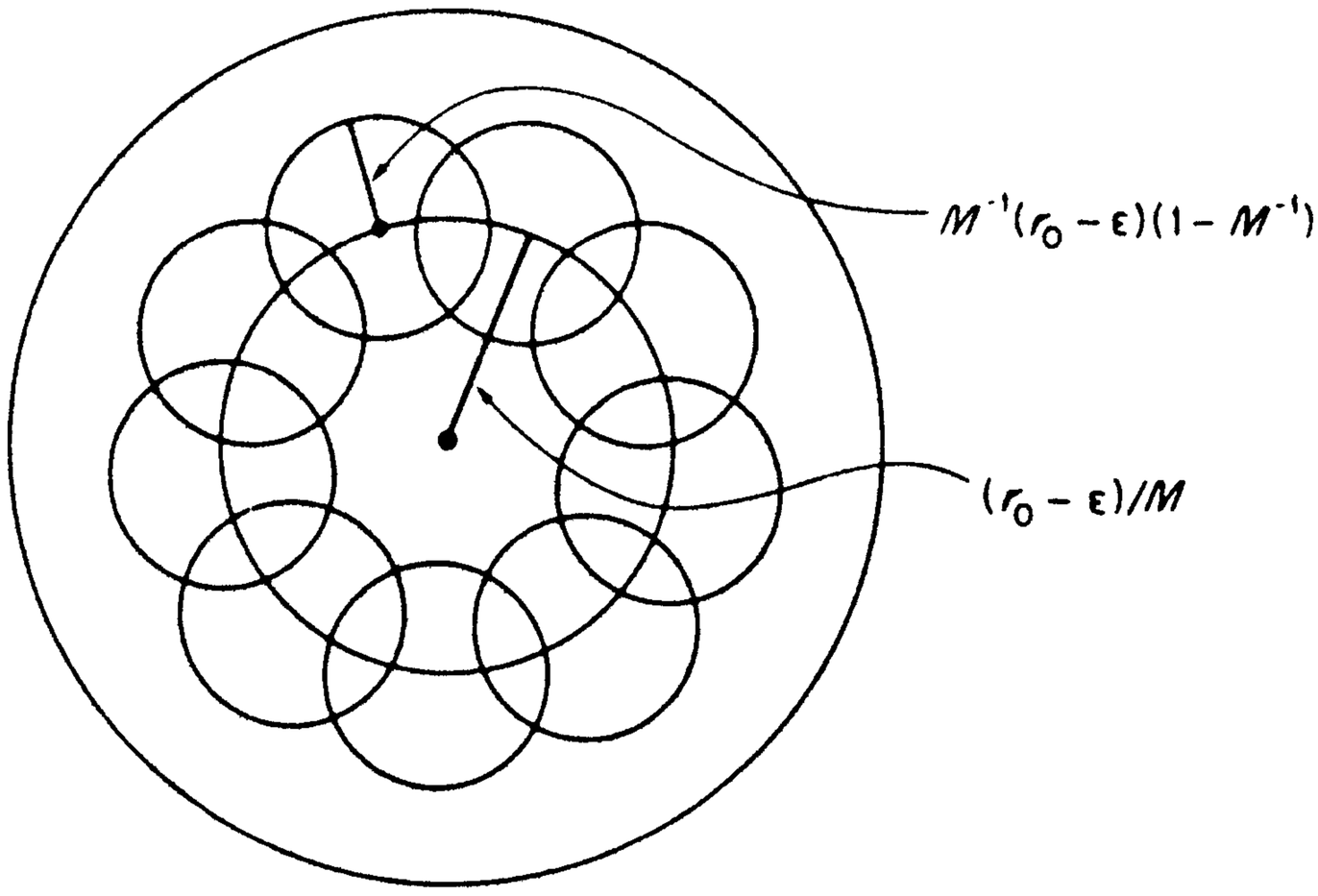


FIGURE XII.1

Proof of Theorem XII.12 We divide the proof into four parts.

(i) Let $Q(\beta) = [P'(\beta), P(\beta)]$. $P^2(\beta) = P(\beta)$, so

$$P'(\beta) = P'(\beta)P(\beta) + P(\beta)P'(\beta) \tag{4}$$

Thus $P(\beta)P'(\beta)P(\beta) = 2P(\beta)P'(\beta)P(\beta)$ or $P(\beta)P'(\beta)P(\beta) = 0$. As a result

$$[Q(\beta), P(\beta)] = P'(\beta)P(\beta) + P(\beta)P'(\beta) - 2P(\beta)P'(\beta)P(\beta) = P'(\beta)$$

by (4).

(ii) Using the lemma with $X = \mathscr{L}(\mathscr{H})$, solve $dU/d\beta = Q(\beta)U(\beta)$ and $dV/d\beta = -V(\beta)Q(\beta)$ with initial conditions $U(0) = 1 = V(0)$. Then $U(\beta)V(\beta) = V(\beta)U(\beta) = 1$; in particular, $U(\beta)$ is invertible. For

$$\frac{d}{d\beta}(V(\beta)U(\beta)) = \frac{dV}{d\beta}U(\beta) + V(\beta)\frac{dU}{d\beta} = 0$$

and thus $VU \equiv 1$. On the other hand, if $F(\beta) = U(\beta)V(\beta)$, then $F(\beta)$ solves the differential equation $dF/d\beta = Q(\beta)F(\beta) - F(\beta)Q(\beta)$; $F(0) = 1$. Since $F(\beta) \equiv 1$ solves this equation with initial condition, we conclude that $F(\beta) = 1$ by the uniqueness of solutions proven in the lemma.

(iii) $U(\beta)P(0)V(\beta) = P(\beta)$. For let $\tilde{P}(\beta) = U(\beta)P(0)V(\beta)$. Then $d\tilde{P}(\beta)/d\beta = [Q(\beta), \tilde{P}(\beta)]$ with initial condition $\tilde{P}(0) = P(0)$. On the other hand, by step (i), $P(\beta)$ also solves $dP(\beta)/d\beta = [Q(\beta), P(\beta)]$ with $P(\beta)|_{\beta=0} = P(0)$. By the uniqueness of solutions of differential equations, $\tilde{P}(\beta) = P(\beta)$.

(iv) Finally, we must prove that $U(\beta)$ is unitary for β real if $P(\beta)$ is self-adjoint for β real. Thus, let us suppose that $P(\beta)^* = P(\beta)$ if $\beta = \bar{\beta}$. By the Schwarz reflection principle, it follows that $P(\beta)^* = P(\bar{\beta})$ for all β. By the definition of Q, $Q(\beta)^* = -Q(\bar{\beta})$. Let $\tilde{V}(\beta) = U(\bar{\beta})^*$. Then $\tilde{V}$ obeys

$d\tilde{V}/d\beta = -\tilde{V}(\beta)Q(\beta)$; $\tilde{V}(0) = I$. By the uniqueness of solutions of differential equations, $\tilde{V}(\beta) = V(\beta)$. Thus, for β real, $U(\beta)^* = \tilde{V}(\beta) = V(\beta) = U(\beta)^{-1}$, so U is unitary. ∎

XII.3 Asymptotic perturbation theory

The elegant regular perturbation theory developed in the preceding section is not always applicable, even to simple-looking examples. Consider the family of Hamiltonians $H(\beta) = H_0 + \beta V$ where $\mathscr{H} = L^2(\mathbb{R})$, $H_0 = -d^2/dx^2 + x^2$, and $V = x^4$. We discussed the self-adjointness of this family from several points of view in Chapter X. For any $\beta > 0$, $H(\beta)$ is self-adjoint on $D(H_0) \cap D(V) = D(p^2) \cap D(x^4)$; see Problem 23 of Chapter X. Since $D(H_0) = D(p^2) \cap D(x^2)$, we see that the domain changes as soon as the perturbation is turned on. Thus the analyticity criterion of Theorem XII.9 is not applicable. A similar change occurs in the form domain $Q(H(\beta))$. In fact, no analyticity criterion can hold since the perturbation series about $\beta = 0$ *diverges.*

The following argument has been made by various authors to predict this divergence of the perturbation series for the eigenvalues of $H(\beta)$ for $\beta \neq 0$: If β is negative, then $x^2 + \beta x^4 \to -\infty$ as $x \to \pm\infty$, so $H_0 + \beta V$ is qualitatively very different from H_0 (it is actually not even essentially self-adjoint). For this reason, one expects that the perturbation series should diverge for β negative. Since power series converge in circles, the series should not converge for any β. Whether or not one wants to accept this heuristic argument, its conclusion is correct. A detailed analysis allows one to prove that the Rayleigh–Schrödinger coefficients a_n for $E_0(\beta)$, the ground state energy, obey $|a_n| \geq AB^n\Gamma(n/2)$ for suitable constants A and B.

Thus, one is faced with deciding whether the perturbation series makes any sense in this case. It is precisely this question that we consider in this section and the next. The meaning of divergent perturbation series is of interest in a wider area than the realm of nonrelativistic quantum mechanics. The most useful calculational tool in certain (at present ill-defined) quantum field theories is another perturbation series known as the Gell'Mann–Low series or Feynman series. In some cases these series have been proven to diverge and they are believed to be divergent in others. For this reason and especially since there are formal similarities between some field theory Hamiltonians and $p^2 + x^2 + \beta x^4$ (see Section X.7), the problems we study in these two sections are relevant to quantum field theory.

The simplest interpretation of a formal series is as an asymptotic series:

Definition Let f be a function defined on the positive real axis. We say that $\sum_{n=0}^{\infty} a_n z^n$ is **asymptotic** to f as $z \downarrow 0$ if and only if, for each fixed N,

$$\lim_{z \downarrow 0} \left(f(z) - \sum_{n=0}^{N} a_n z^n \right) \Big/ z^N = 0$$

If f is defined in a sectorial region of the complex plane $\{z \mid 0 < |z| < B; |\arg z| \leq \theta\}$, we say that $\sum a_n z^n$ is **asymptotic** to f as $|z| \to 0$ **uniformly in the sector** if, for each N,

$$\lim_{\substack{|z| \to 0 \\ |\arg z| \leq \theta}} \left(f(z) - \sum_{n=0}^{N} a_n z^n \right) \Big/ z^N = 0$$

If $\sum a_n z^n$ is asymptotic to f, we shall sometimes write

$$f \underset{z \downarrow 0}{\sim} \sum a_n z^n$$

Notice that if $f \sim \sum a_n z^n$ and $f \sim \sum b_n z^n$ as $z \downarrow 0$, then

$$\lim_{z \downarrow 0} \left(\sum_{n=0}^{N} a_n z^n - \sum_{n=0}^{N} b_n z^n \right) \Big/ z^N = 0$$

for all N, so $a_n = b_n$ for all n. Thus, *any function f has at most one asymptotic series as $z \downarrow 0$.*

Example 1 Consider the function $f(z) = \exp(-z^{-1})$ for $z > 0$. Then $z^{-n} f(z) \to 0$ as $z \downarrow 0$, so f has zero asymptotic series. In fact, the zero series is asymptotic uniformly in any sector $|\arg z| \leq \theta$ with $\theta < \pi/2$.

This example illustrates an important fact about asymptotic series: *Two different functions may have the same asymptotic series.* Saying that f has a certain asymptotic series gives us no information about the value of $f(z)$ for some fixed nonzero value of z. We know that $f(z)$ is well approximated by $a_0 + a_1 z$ as z gets "small," but the definition says nothing about how small is "small." If an asymptotic series $\sum_{n=0}^{\infty} a_n z^n$ is not convergent, the typical behavior is the following: If z is "small," the first few partial sums are a fairly good approximation to $f(z)$, but as $N \to \infty$, the sums oscillate wildly and no longer approximate f very well. For example, we shall presently show that the Rayleigh–Schrödinger series for $E_0(\beta)$, the ground state energy of the Hamiltonian, $p^2 + x^2 + \beta x^4$ $(\beta > 0)$, is asymptotic to $E_0(\beta)$ as $\beta \downarrow 0$. For

$\beta = 0.2$, variational methods (see Section XIII.2) show that $E_0(\beta) = 1.118292\ldots$. The first 15 partial sums are given in the accompanying tabulation.

N	$\sum_{n=0}^{N} a_n(0.2)^n$	N	$\sum_{n=0}^{N} a_n(0.2)^n$
1	1.150000	9	2.353090
2	1.097500	10	−2.442698
3	1.153750	11	13.253968
4	1.105372	12	−42.333586
5	1.176999	13	168.895730
6	1.049024	14	−796.466406
7	1.314970	15	3005.179546
8	0.686006		

Thus, we see the typical behavior of wandering near the right answer for a while (and not even that near!) and then going wild. And as N gets larger, things get worse: The 50th partial sum is about 10^{45} in magnitude and the 1000th about 10^{2000} in magnitude.

Example 2 Let f be C^∞ on $[-1, 1]$. Then $\sum_{n=0}^{\infty} (f^{(n)}(0)/n!)x^n$ is asymptotic as $x \downarrow 0$ or $x \uparrow 0$ to f. For Taylor's theorem with a remainder says that

$$\left| f(x) - \sum_{n=0}^{N} \frac{f^{(n)}(0)}{n!} x^n \right| \leq \frac{|x|^{N+1}}{(N+1)!} \sup_{|a| \leq |x|} [\,|f^{(n+1)}(a)|\,]$$

Since C^∞ functions can be nonanalytic, this example shows that asymptotic series may not converge; and even if they do, the sum may not have anything to do with the function f (see Example 1).

We defined analytic families on open sets. We will abuse this terminology by saying that a family is analytic on a closed set if it is norm continuous on the set and analytic in the interior.

Theorem XII.14 Let H_0 be a self-adjoint operator. Suppose that $H(\beta)$ is an analytic family in the region $\{\beta \,|\, 0 < |\beta| < B;\ |\arg \beta| \leq \theta\}$ and that the following conditions are obeyed:

(a) $\lim_{\substack{|\beta| \to 0 \\ |\arg \beta| \leq \theta}} \|(H(\beta) - \lambda)^{-1} - (H_0 - \lambda)^{-1}\| = 0$ for some $\lambda \notin \sigma(H_0)$.

(b) There is a closed symmetric operator V so that $C^\infty(H_0) \subset D(V)$ and $V[C^\infty(H_0)] \subset C^\infty(H_0)$.
(c) $C^\infty(H_0) \subset D(H(\beta))$ for all β in the sector and for $\psi \in C^\infty(H_0)$, $H(\beta)\psi = H_0\psi + \beta V\psi$.

Let E_0 be an isolated nondegenerate eigenvalue of H_0. Then if $|\beta|$ is small and $|\arg \beta| \leq \theta$, there is exactly one eigenvalue $E(\beta)$ of $H(\beta)$ near E_0. Moreover, the formal Rayleigh–Schrödinger series $\sum a_n \beta^n$ for the eigenvalue of $H_0 + \beta V$ is finite term by term and is an asymptotic series for $E(\beta)$ uniformly in the sector. Explicitly,

$$\lim_{\substack{|\beta| \to 0 \\ |\arg \beta| \leq \theta}} \left| E(\beta) - \sum_{n=0}^{N} a_n \beta^n \right| \Big/ \beta^N = 0$$

for all N.

This is the main result of this section. The conclusion makes several distinct statements, and for this reason we divide the proof into several lemmas. The first conclusion states that there is an eigenvalue $E(\beta)$ of $H_0 + \beta V$ near E_0 if β is small. We shall emphasize this property by giving it a name (stability). In Sections 5 and 6 we discuss situations where such stability does not hold. The second part of the conclusion concerns the asymptotic nature of the perturbation series for $E(\beta)$. A similar result holds for the eigenvector associated with $E(\beta)$ (see Problem 24). The main tool used in establishing the asymptotic property is familiar from Section 2: We use the formulas

$$E(\beta) = \frac{(\Omega_0\,,\,(H_0 + \beta V)P(\beta)\Omega_0)}{(\Omega_0\,,\,P(\beta)\Omega_0)}$$

and

$$P(\beta) = -\frac{1}{2\pi i} \oint (H(\beta) - E)^{-1}\, dE$$

As we have seen, these formulas allow one to unravel the complicated structure of the Rayleigh–Schrödinger coefficients into several simple operations on a geometric series. Our main tool will be the well-known error term for this series.

Definition Let $A(\beta)$ be a family of operators in the set $\{\beta | 0 < |\beta| < B, |\arg \beta| \leq \theta\}$. Suppose that an operator A_0 exists so that for some $\lambda \notin \sigma(A_0)$,

$$\text{s-lim}_{\substack{|\beta| \to 0 \\ |\arg \beta| \leq \theta}} (A(\beta) - \lambda)^{-1} = (A_0 - \lambda)^{-1}$$

An isolated nondegenerate eigenvalue E_0 of A_0 is called **stable** if $A(\beta)$ has exactly one eigenvalue near E_0 for β small and that eigenvalue is isolated and nondegenerate. Thus, E_0 is stable if, for all sufficiently small ε, there is a δ so that $|\beta| < \delta$ and $|\arg \beta| \leq \theta$ imply that there is exactly one point of $\sigma(A(\beta))$ in $\{E \mid |E - E_0| \leq \varepsilon\}$ and that point is a nondegenerate eigenvalue.

Lemma 1 If hypothesis (a) of Theorem XII.14 holds, then any isolated nondegenerate eigenvalue of H_0 is stable.

Proof An application of the first resolvent formula shows that if $(H(\beta) - \lambda)^{-1} \to (H_0 - \lambda)^{-1}$ in norm for some $\lambda \notin \sigma(H_0)$, it converges for all $\lambda \notin \sigma(H_0)$ and the convergence is uniform on compact sets of $\rho(H_0)$. Thus if ε is given so that H_0 has only one eigenvalue in $\{E \mid |E - E_0| \leq \varepsilon\}$, then for some δ, we conclude that $E \notin \sigma(H(\beta))$ if $|\beta| \leq \delta$, $|\arg \beta| \leq \theta$, and $|E - E_0| = \varepsilon$. Therefore, for $|\beta|$ small,

$$P(\beta) = -(2\pi i)^{-1} \oint_{|E-E_0|=\varepsilon} (H(\beta) - E)^{-1}\, dE$$

exists and converges in norm to

$$P_0 = -(2\pi i)^{-1} \oint_{|E-E_0|=\varepsilon} (H_0 - E)^{-1}\, dE$$

as $|\beta| \to 0$. By Theorem XII.5, P_0 is the projection onto the eigenvector of H_0 with eigenvalue E_0. By the lemma preceding Theorem XII.8, $P(\beta)$ is one dimensional if $|\beta|$ is small. Thus Lemma 1 follows from Theorem XII.6. ∎

Next we develop an asymptotic series for $P(\beta)\Omega_0$:

Lemma 2 Suppose that the hypotheses of Theorem XII.14 hold and that Ω_0 is the eigenvector of H_0 with eigenvalue E_0. For $|\beta|$ small, let $\Omega(\beta) = P(\beta)\Omega_0$ with $P(\beta)$ given as above. Then, for all N,

$$\lim_{\substack{|\beta|\to 0 \\ |\arg\beta|\leq\theta}} \left\| \Omega(\beta) - \sum_{n=0}^{N} \varphi_n \beta^n \right\| \Big/ |\beta|^N = 0$$

where

$$\varphi_n = (-1)^{n+1}(2\pi i)^{-1} \oint_{|E-E_0|=\varepsilon} (H_0 - E)^{-1}[V(H_0 - E)^{-1}]^n \Omega_0\, dE$$

Proof Let $|E - E_0| = \varepsilon$. Formally,

$$(H(\beta) - E)^{-1} = \sum_{n=0}^{N} (-\beta)^n (H_0 - E)^{-1}[V(H_0 - E)^{-1}]^n + (-\beta)^{N+1}(H(\beta) - E)^{-1}[V(H_0 - E)^{-1}]^{N+1}$$

Consider applying both sides of this formal equation to Ω_0. Since $\Omega_0 \in C^\infty(H_0)$, both sides are well defined by condition (b). By condition (c), both sides give the same result when $H(\beta) - E$ is applied. Since $E \notin \sigma(H(\beta))$, the two sides are equal. By using the closed graph theorem, one can prove that $[V(H_0 - E)^{-1}]^N \Omega_0$ is continuous in E on $\{E \mid |E - E_0| = \varepsilon\}$ (see Problem 25). Thus,

$$\left\| \Omega(\beta) - \sum_{n=0}^{N} \varphi_n \beta^n \right\| \Big/ |\beta|^N$$

$$= \frac{|\beta|}{2\pi} \left\| \oint_{|E-E_0|=\varepsilon} (H(\beta) - E)^{-1}[V(H_0 - E)^{-1}]^{N+1}\Omega_0 \, dE \right\|$$

$$\leq \varepsilon |\beta| \sup_{\substack{|E-E_0|=\varepsilon \\ |\beta|<\delta \\ |\arg \beta| \leq \theta}} \|(H(\beta) - E)^{-1}\| \, \|[V(H_0 - E)^{-1}]^{N+1}\Omega_0\|$$

$$\to 0 \quad \text{as} \quad |\beta| \to 0 \ \blacksquare$$

To conclude the proof of the theorem, we need the following lemma whose proof is left to Problem 26c.

Lemma 3 Let f and g be two functions defined in the sector $\{\beta \mid 0 < |\beta| < B;\ |\arg \beta| \leq \theta\}$. Suppose that $f \sim_{\beta \to 0} \sum a_n \beta^n$ and $g \sim_{\beta \to 0} \sum b_n \beta^n$ with $b_0 \neq 0$. Let $\sum c_n \beta^n$ be the formal series for $\sum a_n \beta^n / \sum b_n \beta^n$. Then the function $h(\beta) = f(\beta)/g(\beta)$ is asymptotic to $\sum c_n \beta^n$ as $\beta \to 0$.

Proof of Theorem XII.14 Since Lemma 1 has been proven, all that remains is to prove that the Rayleigh–Schrödinger series is finite term by term and asymptotic. By Lemma 2 and hypothesis (b), the series for $(H(\beta)\Omega_0, P(\beta)\Omega_0)$ and $(\Omega_0, P(\beta)\Omega_0)$ are finite term by term and asymptotic. Since $\lim_{|\beta| \to 0} (\Omega_0, P(\beta)\Omega_0) = 1 \neq 0$, Lemma 3 completes the proof. ∎

Finally we must ask when condition (a) can be proven. Let us state two general theorems. We shall only sketch the proof of one of them (for references, see the Notes). As in Chapter XIII, we will say that two self-adjoint

operators A and B which are bounded from below satisfy $A \leq B$ if $Q(B) \subset Q(A)$ and $(\varphi, A\varphi) \leq (\varphi, B\varphi)$ for all φ in $Q(B)$.

Theorem XII.15 Suppose that H_0 and V are self-adjoint. Suppose, moreover, that:

(i) $H_0 \geq 0$.
(ii) For each $a > 0$, there is a b so that

$$V_- \leq aH_0 + b$$

(V_- is the negative part of V given by the spectral theorem; in particular, if $V \geq 0$, $V_- = 0$ so (ii) holds.)
(iii) For some c and d

$$|V| \leq cH_0^2 + d$$

Then $H_0 + \beta V$ is an analytic family of type (B) in the cut plane $\{\beta \,|\, |\arg \beta| < \pi;\ |\beta| > 0\}$ and

$$\lim_{\substack{|\beta| \to 0 \\ |\arg \beta| \leq \theta}} \|(H(\beta) - \lambda)^{-1} - (H_0 - \lambda)^{-1}\| = 0$$

for any $\theta < \pi$.

Theorem XII.16 Suppose that H_0 and V are self-adjoint operators. Suppose, moreover, that:

(i) $H_0 \geq 0$.
(ii) For each $a > 0$, there is a b so $V_- \leq aH_0 + b$.
(iii) For some d, some $c < 1$, and some B,

$$\pm\beta[H_0^{1/2}, [H_0^{1/2}, V]] \leq c(H_0^2 + \beta^2 V^2) + d \qquad \text{if} \quad 0 < \beta < B$$

(iv) For all $e > 0$, there is an f so that

$$\pm\beta i[H_0\,, V] \leq e(H_0^2 + \beta^2 V^2) + f \qquad \text{if} \quad 0 < \beta < B$$

(v) For some $p > 1$, g, and h,

$$|V|^{2/p} \leq gH_0^2 + h$$

(vi) $H_0 + \beta V$ is essentially self-adjoint on $D(H_0) \cap D(V)$ if $0 < \beta < B$.

Then $H_0 + \beta V$ is an analytic family of type (B) in the cut plane and

$$\lim_{\substack{|\beta| \to 0 \\ |\arg \beta| \leq \theta}} \|(H(\beta) - \lambda)^{-1} - (H_0 - \lambda)^{-1}\| = 0$$

for any $\theta < \pi$.

If in addition:

(iii'), (iv') For any B, we can choose d, f suitably so that the basic estimates in (iii), (iv) hold; and

(vi') $H_0 + \beta V$ is essentially self-adjoint on $D(H_0) \cap D(V)$ for all $\beta > 0$,

then $H(\beta)$ is an analytic family of type (A) in the cut plane.

The main idea of the proof of Theorem XII.16 is to use (ii), (iii), and (iv) to prove "quadratic" estimates. Specifically, given $\theta < \pi$, one can find, α, $\gamma > 0$ so that

$$H_0^2 + |\beta|^2 V^2 \leq \alpha(H_0 + \beta V)^*(H_0 + \beta V) + \gamma$$

for all β with $0 < |\beta| < B$; $|\arg \beta| < \theta$. It then follows that $H_0 + \beta V$ is closed on $D(H_0) \cap D(V)$ (Problem 27). Now write

$$\|(H_0 + \beta V - \lambda)^{-1} - (H_0 - \lambda)^{-1}\|$$

$$\leq |\beta|^{1/p} \|(H(\beta) - \lambda)^{-1} |\beta V|^{1-(1/p)} |V|^{1/p} (H_0 - \lambda)^{-1}\|$$

By the quadratic estimate, $(H(\beta) - \lambda)^{-1} |\beta V|^{1-(1/p)}$ is bounded uniformly in the sector $\{\beta | 0 < |\beta| < B; \ |\arg \beta| < \theta\}$. By (v), $|V|^{1/p}(H_0 - \lambda)^{-1}$ is bounded. Thus $\|(H_0 + \beta V - \lambda)^{-1} - (H_0 - \lambda)^{-1}\|$ goes to zero at least as fast as $|\beta|^{1/p}$.

Example 3 (the anharmonic oscillator) Let $H_0 = -d^2/dx^2 + x^2$ on $L^2(\mathbb{R})$ and $V = x^{2m}$. Then all the conditions of Theorem XII.16 hold. (i) and (ii) are immediate. (vi) was proven in Example 2 of Section X.4 and Example 2 of Section X.9. To prove (iii) and (iv), one does explicit computations with the creation and annihilation operators A, $A^\dagger$, introduced in the Appendix to Section V.3 (see Problem 28). (v) holds with $p = m$ by again using A and $A^\dagger$ (Problem 28). Since V leaves $C^\infty(H_0)$ invariant and Theorem XII.16 is applicable, all the conditions of Theorem XII.14 hold. Thus the eigenvalues of $p^2 + x^2 + \beta x^{2m}$ have Rayleigh–Schrödinger series as asymptotic series, uniformly in sectors $|\arg \beta| \leq \theta < \pi$. It can also be proven that the eigenvalues have analytic continuations onto many-sheeted surfaces, $\arg |\beta| \leq \theta$, $0 < \beta < B_\theta$, for any $\theta < ((m+1)/2)\pi$ where the series is asymptotic on the many-sheeted surface.

Example 4 ($(\varphi^4)_2$ field theory with a spatial cut-off) Let H_0 be the free boson field of mass $m_0 > 0$ in two-dimensional space–time. Let $V = \int g(x) : \varphi^4(x) : dx$ with $g \in L^1 \cap L^2$ and $g \geq 0$ (as discussed in Section

X.7). Then, one can prove all the conditions of Theorem XII.16 (or Theorem XII.15). The only isolated eigenvalue of H_0 is the Fock vacuum. Theorem XII.14 is not applicable in the stated form because $C^\infty(H_0)$ is not invariant under V. However, if N is the number operator, V and $(H_0 - E)^{-1}$ leave $C^\infty(N)$ invariant and $\Omega_0 \in C^\infty(N)$. It is easy to extend the method used in Theorem XII.14 to prove that the Rayleigh–Schrödinger series is asymptotic when the invariance of $C^\infty(H_0)$ is replaced by invariance of $C^\infty(N)$. In this way one can conclude that the ground state energy of $H_0 + \beta V$ has an asymptotic series. The coefficients are given by sums of Feynman type diagrams (see the Notes).

When condition (a) of Theorem XII.14 holds, it is a convenient tool for proving stability, but there are cases where it fails in which stability can be proven by the following method:

Theorem XII.16.5 Let H_0 be a closed operator and P a finite dimensional *orthogonal* projection so that $\operatorname{Ran} P \subset D(H_0)$, and $H_0 P = P H_0$. Suppose that the operator $H_0 \restriction \operatorname{Ran}(1 - P)$ is sectorial with sector $S_0 \equiv \{z \mid |\arg z| \leq \theta_0 < \pi/2\}$ and that $H_0 \restriction \operatorname{Ran} P$ has spectrum outside S_0. Let V be a closed sectorial operator with sector S_0. Suppose that $\operatorname{Ran} P \subset D(V) \cup D(V^*)$. Let E_0 be an isolated nondegenerate eigenvalue of $H_0 \restriction \operatorname{Ran} P$. Then, for any ε, $\delta > 0$, there is a B so that the form sum $H_0 + \beta V$ has exactly one eigenvalue, $E(\beta)$, in $\{E \mid |E - E_0| < \varepsilon\}$ for β in the region $Q \equiv \{\beta \mid |\arg \beta| \leq \pi/2 - \theta_0 - \delta;\ |\beta| \leq B\}$. The eigenvalue is nondegenerate, it is the only spectral point of $H_0 + \beta V$ near E_0, and

$$\sup\{\|(H_0 + \beta V - E)^{-1}\| \mid |E - E_0| = \varepsilon;\ \beta \in Q\} < \infty$$

Moreover, suppose that $H_0 \Omega_0 = E_0 \Omega_0$ and that for $|E - E_0| = \varepsilon$, we have that $((H_0 - E)^{-1} V)^j (H_0 - E)^{-1} \Omega_0 \in D(V)$ for $j = 0, 1, \ldots, k$. Then the Rayleigh–Schrödinger coefficients for $E(\beta)$ are finite up to order at least β^{k+1} and the Rayleigh–Schrödinger series is asymptotic to at least that order in the region Q.

Proof It suffices to prove stability since the asymptotic series result then follows as in the proofs of Lemmas 2 and 3. Write $V = V_1 + V_2$ where $V_1 = (1 - P)V(1 - P)$, $V_2 = V - V_1$. V_2 is a bounded finite rank operator since $\operatorname{Ran} P \subset D(V) \cup D(V^*)$. Clearly, $H_0 + \beta V_1$ is sectorial on $\operatorname{Ran}(1 - P)$ for $\beta \in Q$ no matter what we take for B and δ and it equals H_0 on $\operatorname{Ran} P$. Since βV_2 is bounded, we can study its effect on $\sigma(H_0 + \beta V_1)$ by regular perturbation theory. The result is that for β small the sup in question is finite so the projection $-(2\pi i)^{-1} \int (H_0 + \beta V - E)^{-1}\, dE$ has constant dimension. ∎

Example 5 Let $H_0 = -\Delta + W$ where W is real-valued and $W(x) \to 0$ as $x \to \infty$. Let $V = |x|$ (we could take $V(x) = |x|^n$). In this case $H_0 + \beta V \to H_0$ in strong resolvent sense but not in norm resolvent sense. The convergence cannot be in norm since $(H_0 + \beta V - i)^{-1}$ is compact (see Section XIII.14) but $(H_0 - i)^{-1}$ is not. Thus Theorem XII.14 is not applicable.

If H_0 has negative eigenvalues, we can take P to be the projection onto the corresponding eigenvectors (or those corresponding to the m lowest eigenvectors in which case we add a constant to H_0 to make sure that $H_0 \restriction (1 - P)$ is sectorial with sector S_0). Since the eigenvectors of H_0 fall off exponentially (see Section XIII.11), Ran $P \subset D(V) = D(V^*)$, so the hypotheses of the first part of Theorem XII.16.5 holds. Moreover, under mild hypotheses on W, one can show, using the method of Section XIII.11, that for E near E_0 and a small, $(H_0 - E)^{-1}$ is a bounded map from $\mathscr{H}_a$ to itself where

$$\mathscr{H}_a = \{\psi \mid \|\psi\|_a = \|e^{a|x|}\psi\|_2 < \infty\}$$

Since $\Omega_0 \in \mathscr{H}_a$ for a small and V is bounded from $\mathscr{H}_a$ to $\mathscr{H}_{a/2}$, we can verify the hypotheses of the second part of Theorem XII.16.5 for any k. Thus, the Rayleigh–Schrödinger series is asymptotic to all orders for any β satisfying Re $\beta > 0$. If $\beta < 0$, the eigenvalue is not stable, but the Rayleigh–Schrödinger series is still relevant as we shall see in Section 5.

Finally, we consider an example which shows that one can sometimes prove that a Rayleigh–Schrödinger series is asymptotic even though the eigenvalues are not stable. However, a detailed argument will be required. This example also illustrates, in a dramatic way, the fact that two distinct functions can have the same asymptotic series.

Example 6 (The double well potential) Consider the family of operators on $L^2(\mathbb{R})$:

$$H(\beta) = -d^2/dx^2 + x^2 + 2\beta x^3 + \beta^2 x^4$$

Since the total potential can be written $x^2(1 + \beta x)^2$, we see that for each $\beta \geq 0$, $H(\beta)$ is bounded from below. By the methods of Chapter X, $H(\beta)$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$ and, by the methods of Section XIII.4 or XIII.14, it has a purely discrete spectrum and a complete set of eigenvectors. Although $H(\beta)$ is not linear in β, it is not hard to extend the formulas we have given in Section 1 to obtain formal series for the eigenvalues: one need only use $2\beta x^3 + \beta^2 x^4$ for V in the formulas of Section 1 up to order n and then collect all terms of order β^n. Because $(\Omega_n, (2\beta x^3 + \beta^2 x^4)\Omega_m) = 0$ if $|n - m| > 4$ for the unperturbed eigenvectors Ω_n

of $H(0)$, the sums in the definition of the Rayleigh–Schrödinger series are all finite and so one has a formal series $\sum_{n=0}^{\infty} a_n \beta_n$ for the eigenvectors of $H(\beta)$. Since the problem is invariant under the changes $x \to -x$, $\beta \to -\beta$, we have that $a_{2n+1} = 0$ for all n.

So far, this problem does not seem so different from the anharmonic oscillator of Example 3, and indeed, if the 2 in the $2\beta x^3$ term were replaced by some θ with $-2 < \theta < 2$, then one could prove norm resolvent convergence as $\beta \downarrow 0$. But notice that the total potential vanishes also at $x = -\beta^{-1}$; indeed, if we translate by $-\frac{1}{2}\beta^{-1}$ units we obtain the unitarily equivalent operator

$$\tilde{H}(\beta) = -d^2/dx^2 + \tfrac{1}{16}\beta^{-2} - \tfrac{1}{2}x^2 + \beta^2 x^4$$

Since the potential term in $\tilde{H}(\beta)$ is symmetric under $x \to -x$, it is evident that $H(\beta)$ has two identical wells in its potential, one centered at $x = 0$ and one at $x = -\beta^{-1}$. As a result, for β very small, we expect two eigenvalues near E_0, the ground state energy of $H(0)$, since we can obtain two nearly orthogonal vectors with energy expectation near $E(0)$ by using the ground state $\Omega_0(x)$ for $H(0)$ and its translate $\Omega_0(x + \beta^{-1})$. For this reason, we will label the eigenvalues of $H(\beta)$ for $\beta > 0$ as $E_0(\beta) < E_0'(\beta) < E_1(\beta) < E_1'(\beta) < \cdots$ and corresponding vectors $\Omega_0(x, \beta)$, etc. To avoid confusion, we will only use prime below to distinguish these eigenvalues and *not* for derivatives. E_0, E_1, ... are just the eigenvalues of $\tilde{H}(\beta)$ whose eigenvectors are invariant under $x \to -x$, and E_0', E_1', ... those whose eigenvectors are odd under $x \to -x$. As $\beta \downarrow 0$, we expect both $E_0(\beta)$ *and* $E_0'(\beta)$ to go to E_0; i.e., the eigenvalue E_0 of $H(0)$ is *not* stable. Moreover, one expects that $E_0'(\beta) - E_0(\beta)$ goes to zero extremely fast, namely as $\exp(-a\beta^{-2})$ for suitable a, because of the following argument: The true eigenvectors of $\tilde{H}(\beta)$ are even and odd under $x \to -x$. If one starts at $t = 0$ with a state like $N(\beta)^{-1}[\Omega_0(x, \beta) + \Omega_0'(x, \beta)]$ which is concentrated near $x = 0$, then after a time $t = \pi/(E_0' - E_0)$, the state, moving under the dynamics given by $H(\beta)$, will be concentrated at $x = -\beta^{-1}$; that is, it will tunnel through the barrier between the wells. Thus $E_0'(\beta) - E_0(\beta)$ should be of the same order as the probability for tunnelling and this should be of order $\exp(-d\sqrt{h})$ where d is the width of the barrier, i.e., $1/\beta$, and h is the height of the barrier, i.e., $\frac{1}{16}\beta^{-2}$.

Therefore, our expectation is that the two eigenvalues $E_0(\beta)$ and $E_0'(\beta)$ approach the single eigenvalue E_0 of $H(0)$, and that both have the same Rayleigh–Schrödinger series as asymptotic series. We want to sketch a proof of these facts leaving the details to the reader (Problem 36). The arguments are rather involved and we will use freely tools from Chapter XIII. We will establish three facts: (i) As $\beta \downarrow 0$, both $E_i(\beta)$ and $E_i'(\beta)$

approach $E_i(0) \equiv E_i$ and in particular, there is a β-independent gap between $E_0'(\beta)$ and $E_1(\beta)$ as β goes to zero. (ii) We will prove that $\exp(-a\beta^{-2}) \leq E_0'(\beta) - E_0(\beta) \leq \exp(-b\beta^{-2})$ as $\beta \downarrow 0$ for suitable a and b. (iii) We will show that $E_0(\beta)$ (and thus by (ii), also $E_0'(\beta)$) has the Rayleigh–Schrödinger series as asymptotic series.

As a preliminary to step (i), we consider the operators $H^{\mathrm{D}}(a)$ and $H^{\mathrm{N}}(a)$ on $L^2(-a, a)$ given by $-d^2/dx^2 + x^2$ with Dirichlet (respectively, Neumann) boundary conditions at $x = \pm a$. Let $E_n^{\mathrm{D}}(a)$ and $E_n^{\mathrm{N}}(a)$ denote the eigenvalues of $H^{\mathrm{D}}(a)$ and $H^{\mathrm{N}}(a)$. Let E_n denote the eigenvalues of $-d^2/dx^2 + x^2$ on all of $L^2(\mathbb{R})$. By the method of Section XIII.15, we have

$$E_n^{\mathrm{N}}(a) \leq E_n \leq E_n^{\mathrm{D}}(a) \tag{5a}$$

so long as $a^2 \geq E_n = 2n + 1$. (This condition is needed so that after Neumann conditions are imposed at $x = \pm a$ on the problem for $L^2(\mathbb{R})$, the lowest eigenvalues for the intervals $|x| \geq a$ are above E_n.) We will show that

$$E_n^{\mathrm{D}}(a) \leq E_n^{\mathrm{N}}(a) + \exp(-ca^2) \tag{5b}$$

for a large, where how large will depend on n. Let $\psi_n^{\mathrm{N}}(x; a)$ denote the nth normalized eigenvector of $H^{\mathrm{N}}(a)$. We claim that for a sufficiently large,

$$|\psi_n^{\mathrm{N}}(a; a)| \leq \exp(-\tfrac{1}{12}a^2) \tag{6}$$

To prove (6), let $\varphi(x)$ solve $-\varphi'' + x^2\varphi = E_n^{\mathrm{N}}(a)\varphi$ with boundary conditions $\varphi'(a) = 0$, $\varphi(a) = 1$. Choose a so large that $a > 16$ and $(a/2)^2 \geq (a^2/9) + (2n + 1)$; then in the interval $[\frac{1}{2}a, a]$, we have $x^2 - E_n^{\mathrm{N}}(a) \geq a^2/9$ since $E_n^{\mathrm{N}}(a) \leq 2n + 1$. Thus, by a comparison argument of the type used in Section XI.2, $\varphi(x) \geq \cosh(\frac{1}{3}a)(x - a))$ for x in $[\frac{1}{2}a, a]$. In particular, $\varphi(x) \geq \frac{1}{2}\exp(\frac{1}{12}a^2)$ for $x \in [\frac{1}{2}a, \frac{3}{4}a]$, and thus, since $a > 16$,

$$\int_{a/2}^{3a/4} |\varphi(x)|^2\, dx \geq \cosh(\tfrac{1}{6}a^2)$$

Since $\psi_n^{\mathrm{N}}(x, a)$ is a normalized multiple of φ, (6) holds. For later purposes, we note that a similar argument shows that

$$\left|\frac{\partial \psi_n^{\mathrm{D}}}{\partial x}(a; a)\right| \leq \exp(-ca^2) \tag{6'}$$

Now fix n_0 and pick a_0 so that (6) holds for $n = 0, \ldots, n_0$ and $a \geq a_0$. Let

$$\eta_i(x) = \begin{cases} \psi_i^{\mathrm{N}}(x, a) - \psi_i^{\mathrm{N}}(a, a) & i = 0, 2, \ldots \\ \psi_i^{\mathrm{N}}(x, a) - a^{-1}x\psi_i^{\mathrm{N}}(a, a) & i = 1, 3, \ldots \end{cases}$$

Then the η_i vanish at $x = \pm a$, so they are suitable trial functions for $H^{\mathrm{D}}(a)$; i.e., they lie in $Q(H^{\mathrm{D}}(a))$. On account of (6), $\Delta_{ij} = (\eta_i, \eta_j)$ and $E_{ij} = (\eta_i, H^{\mathrm{D}}(a)\eta_j)$ obey, for $0 \leq i, j \leq n_0$:

$$|\Delta_{ij} - \delta_{ij}| \leq d \exp(-\tfrac{1}{20} a^2)$$

$$|E_{ij} - E_i^{\mathrm{N}}(a)\delta_{ij}| \leq d \exp(-\tfrac{1}{20} a^2)$$

for d suitable. Let $E_{(i)}$ be the ith eigenvalue of $\Delta^{-1/2} E \Delta^{-1/2}$ where $\Delta = \{\Delta_{ij}\}$ and $E = \{E_{ij}\}$. By the Rayleigh–Ritz method of Section XIII.2, $E_{(i)} \geq E_i^{\mathrm{D}}(a)$ (for $i = 0, \ldots, n_0$) and by the above,

$$\|\Delta^{-1/2} E \Delta^{-1/2} - E_i^{\mathrm{N}} \delta_{ij}\| \leq d_1 \exp(-\tfrac{1}{20} a^2)$$

It follows that $|E_{(i)} - E_i^{\mathrm{N}}| \leq d_1 \exp(-\frac{1}{20} a^2)$ so that (5b) holds.

We can now accomplish step (i). By the form of $\tilde{H}(\beta)$, E_i (respectively, E_i') is the $(i+1)$st eigenvalue of $-d^2/dx^2 + x^2 + 2\beta x^3 + \beta^2 x^4$ on $L^2(-\frac{1}{2}\beta^{-1}, \infty)$ with Neumann (respectively, Dirichlet) boundary condition at $x = -\frac{1}{2}\beta^{-1}$. Fix $a > \sqrt{2n+1}$, and put additional Dirichlet or Neumann boundary conditions at $x = \pm a$. Let $E_{i,\,\mathrm{D}}(\beta, a)$, $E_{i,\,\mathrm{N}}(\beta, a)$, $E'_{i,\,\mathrm{D}}(\beta, a)$, $E'_{i,\,\mathrm{N}}(\beta, a)$ denote the corresponding eigenvalues. By Dirichlet–Neumann bracketing (Section XIII.15),

$$E_{i,\,\mathrm{N}}(\beta, a) \leq E_i(\beta) \leq E_{i,\,\mathrm{D}}(\beta, a)$$

and similarly for the primed quantities. Taking β to zero we see that

$$E_i^{\mathrm{N}}(a) \leq \underline{\lim}\, E_i(\beta) \leq \overline{\lim}\, E_i(\beta) \leq E_i^{\mathrm{D}}(a)$$

where $E_i^{\mathrm{N}}(a)$ is as defined in the last paragraph. Taking now $a \to \infty$ and using (5), we see that $|E_i(\beta) - E_i| \to 0$ as $\beta \to 0$.

As a preliminary to step (ii), we note that as $\beta \downarrow 0$, $\|\Omega_i(\beta) - \tilde{\Omega}_i(\beta)\| \to 0$ and $\|\Omega_i'(\beta) - \tilde{\Omega}_i'(\beta)\| \to 0$ where $\tilde{\Omega}_i(x, \beta) = 2^{-1/2}(\Omega_i(x) + \Omega_i(x + \beta^{-1}))$ and $\tilde{\Omega}_i'(x, \beta) = 2^{-1/2}(\Omega_i(x) - \Omega_i(x + \beta^{-1}))$. For $\tilde{\Omega}_i$ is even under reflection about $x = -\frac{1}{2}\beta^{-1}$ and

$$\|(H(\beta) - E_i(\beta))\tilde{\Omega}_i\| \to 0$$

as $\beta \downarrow 0$. Since $H(\beta)$ has only one eigenvalue with an even eigenvector near $E_i(\beta)$ we have that $\|\Omega_i(\beta) - \tilde{\Omega}_i(\beta)\| \to 0$. The argument with primes is similar. In particular,

$$\int_{-\frac{1}{2}\beta^{-1}}^{\infty} \Omega_i(x, \beta)\Omega_i'(x, \beta)\, dx \to \tfrac{1}{2} \tag{7}$$

as $\beta \downarrow 0$.

Using (7), the boundary conditions at $x = -\frac{1}{2}\beta^{-1}$, and an integration by parts in

$$\int_{-\frac{1}{2}\beta^{-1}}^{\infty} [\Omega_i(H(\beta)\Omega_i') - \Omega_i'(H(\beta)\Omega_i)]\, dx$$

one finds that

$$\tfrac{1}{2}(E_i' - E_i) = \Omega_i(-\tfrac{1}{2}\beta^{-1}, \beta)\frac{d}{dx}\Omega_i'(-\tfrac{1}{2}\beta^{-1}, \beta) \tag{8}$$

By the method used in the proof of (6) and (6′) and the fact that on $(-\frac{1}{2}\beta^{-1}, 0)$, we have $\frac{1}{4}x^2 \leq x^2(1+\beta x)^2 \leq x^2$, it is easy to show that the right side of (8) is bounded below by $\exp(-a\beta^{-2})$ and above by $\exp(-b\beta^{-2})$. This completes the proof of step (ii).

Finally we turn to step (iii). For $\varphi \in \mathscr{S}$, it is easy to see that $(H(\beta) - H(0))\varphi \to 0$ as $\beta \downarrow 0$. Since the spectrum of $H(\beta)$ approaches that of $H(0)$ by step (i), we see that $(H(\beta) - z)^{-1} - (H(0) - z)^{-1} \to 0$ strongly as $\beta \downarrow 0$ for $z \neq 2n + 1$. In particular, if

$$P(\beta) = (2\pi i)^{-1} \int_{|z-1|=1/2} (z - H(\beta))^{-1}\, dz$$

then $P(\beta) \to P(0)$ strongly as $\beta \downarrow 0$. Of course $P(0)$ is a rank 1 projection and $P(\beta)$ for $\beta \neq 0$ is a rank 2 projection. As usual $e(\beta) \equiv (\Omega_0, P(\beta)\Omega_0)^{-1}$ $(\Omega_0, H(\beta)P(\beta)\Omega_0)$ has the Rayleigh–Schrödinger series as asymptotic series. Moreover, $e(\beta) = \theta(\beta)\, E_0(\beta) + (1 - \theta(\beta))E_0'(\beta)$ for a suitable function $\theta(\beta)$. Since $E_0 - E_0' \to 0$ faster than any power, both $E_0(\beta)$ and $E_0'(\beta)$ have the same Rayleigh–Schrödinger series as asymptotic series.

XII.4 Summability methods in perturbation theory

The idea that a function could be determined by a divergent asymptotic series was a foreign one to the nineteenth century mind. Borel, when an unknown young man, discovered that his summability method yielded the "right" answer for many classical divergent series. He decided to make a pilgrimage to Stockholm to see Mittag-Leffler, who was the recognized lord of complex analysis. Mittag-Leffler listened politely to what Borel had to say and then, placing his hand upon the complete works of Weierstrass, his teacher, he said, in Latin, "The Master forbids it."

A tale of Mark Kac

We have just seen that a divergent perturbation series such as the one for energy levels of $p^2 + x^2 + \beta x^4$ can nonetheless give some information about the actual energy levels and that under fairly general circumstances, the

Rayleigh–Schrödinger series is an asymptotic series. We also saw that saying a series is an asymptotic series is a very weak statement; in particular, saying that $\sum_{n=0}^{\infty} a_n \beta^n$ is asymptotic for $E(\beta)$ gives one no information about $E(\beta_0)$ for fixed $\beta_0 \neq 0$. In this section, we shall study the question of whether, nevertheless, the divergent perturbation series might determine the energy level $E(\beta)$ by some method more subtle than direct summation.

We first seek some condition stronger than saying that $\sum_{n=0}^{\infty} a_n \beta^n$ is asymptotic to $E(\beta)$, and weaker than saying the sum is convergent, but that determines $E(\beta)$ uniquely. Recall that the nonuniqueness associated with asymptotic series came from the fact that nonzero functions like $\exp(-\beta^{-1})$ could have a zero asymptotic series. We thus seek a stronger condition that guarantees uniqueness. Such a condition is supplied by the following theorem of Carleman:

Theorem XII.17 (Carleman's theorem) Let g be a function analytic in the interior of $S = \{z | 0 \leq |z| \leq B;\ |\arg z| \leq \pi/2\}$ and continuous on S. Suppose that for each n,

$$|g(z)| \leq b_n |z|^n$$

for all z in the sector. If moreover $\sum_{n=1}^{\infty} b_n^{-1/n} = \infty$, then g is identically zero.

In applications, we need only the special case of Carleman's theorem proven below. We remark that the condition $|g(z)| \leq b_n |z|^n$ says exactly that g has 0 asymptotic series. The additional condition $\sum_{n=1}^{\infty} b_n^{-1/n} = \infty$ is a bound on how quickly $b_n^{-1/n}$ can go to zero or equivalently how fast b_n can go to infinity. Since $\sum_{n=1}^{\infty} n^{-1}$ is barely divergent, $\sum_{n=1}^{\infty} b_n^{-1/n} = \infty$ is only slightly weaker than a bound $b_n \leq C_0 B_0^n n^n$ for suitable C_0, B_0 or equivalently $b_n \leq CB^n n!$, for suitable C, B. We prove the following special case of Carleman's theorem:

Theorem XII.18 Suppose that g is a function analytic in the interior of and continuous on $S = \{z | |\arg z| \leq \frac{1}{2}\pi + \varepsilon; 0 < |z| \leq R\}$ for some $\varepsilon > 0$. If there exist C and B so that

$$|g(z)| \leq CB^n n!\ |z|^n$$

for all $z \in S$ and all n, then g is identically zero.

Proof For simplicity of notation, let $w = z^{-1}$ and $f(w) = g(w^{-1})$. Then f is analytic in

$$\tilde{S} = \{w | |\arg w| \leq \tfrac{1}{2}\pi + \varepsilon;\ |w| \geq R^{-1}\}$$

For all n, $|f(w)| \leq CB^n n! \, |w|^{-n}$ for all w in $\tilde{S}$. By Stirling's formula, for any $\delta > 0$ we can find D_δ so that $n! \leq D_\delta n^n e^{-n(1-\delta)}$. Taking n to be the largest integer less than $|w|/B$, we see $|f(w)| \leq C' e^{-\varepsilon|w|}$ for some C' and ε. Using a technique known as the Phragmén–Lindelöf principle, we shall show that $f(w_0) = 0$ if w_0 is real and $w_0 > R^{-1}$ and conclude that $f \equiv 0$ by analytic continuation. Pick α so that $\alpha(\frac{1}{2}\pi + \varepsilon) = \frac{1}{2}\pi$. Let $f_m(w) = f(w) \exp[m(w/w_0)^\alpha]$. Since $\alpha < 1$ and $|f(w)| \leq C' e^{-\varepsilon|w|}$, $f_m(w) \to 0$ as $|w| \to \infty$. Thus, by the maximum principle,

$$|f_m(w_0)| \leq \max\{|f_m(w)| \, | \, |w| = R^{-1} \quad \text{or} \quad |\arg w| = \tfrac{1}{2}\pi + \varepsilon\}$$

Letting $M_1 = \max\{|f(w)| \, | \, |w| = R^{-1}\}$ and $M_2 = \max\{|f(w)| \, | \, |\arg w| = \frac{1}{2}\pi + \varepsilon\}$ we see that

$$|f_m(w_0)| \leq \max\{M_1 \exp[m(R^{-1}/w_0)^\alpha], M_2\}$$

so that

$$|f(w_0)| \leq \max\{M_1 \exp[m(-1 + (R^{-1}/w_0)^\alpha)], M_2 \exp[-m]\}$$

Since m is arbitrary, $f(w_0) = 0$. ∎

In the proof just given we established that if f is analytic in $\tilde{S}$ with exponential falloff, then f is zero. We shall prove and use an extension of this fact (Carlson's theorem) in Section XIII.13.

This last theorem suggests that we single out a stronger condition than the statement that $E(\beta)$ has $\sum_{n=0}^{\infty} a_n \beta^n$ as asymptotic series.

Definition We say that a function $E(\beta)$, analytic in a sectorial region $\{\beta \,|\, 0 < |\beta| < B; \ |\arg \beta| < \frac{1}{2}\pi + \varepsilon\}$, obeys a **strong asymptotic condition** and has $\sum_{n=0}^{\infty} a_n \beta^n$ as **strong asymptotic series** if there are C and σ so that

$$\left| E(\beta) - \sum_{n=0}^{N} a_n \beta^n \right| \leq C\sigma^{N+1}(N+1)! \, |\beta|^{N+1}$$

for all N and all β in the sector.

Theorem XII.19 If $\sum_{n=0}^{\infty} a_n \beta^n$ is a strong asymptotic series for two analytic functions f and g, then $f = g$.

Proof By hypothesis,

$$|f(\beta) - g(\beta)| \leq 2C\sigma^{N+1}(N+1)! \, |\beta|^{N+1}$$

in $\{\beta \,|\, 0 < |\beta| \leq \frac{1}{2}B; \ |\arg \beta| \leq \frac{1}{2}\pi + \frac{1}{2}\varepsilon\}$, so Theorem XII.18 implies that $f - g = 0$. ∎

To apply the idea of strong asymptotic conditions to eigenvalues it is useful to have the following simple technical lemma (Problem 26).

Lemma If f and g obey strong asymptotic conditions and if $\lim_{|\beta|\to 0} g(\beta) \neq 0$, then f/g obeys a strong asymptotic condition with asymptotic series given by the formal quotient of the asymptotic series for f and g.

Example 1 Consider the energy levels of the anharmonic oscillator $p^2 + x^2 + \beta x^4$. We have seen that $E(\beta) = (H(\beta)\Omega_0, P(\beta)\Omega_0)/(\Omega_0, P(\beta)\Omega_0)$. By the preceding lemma, it is sufficient to get a bound of the form $C\sigma^{N+1}(N+1)!\,|\beta|^{N+1}$ on the norm of the remainder of $P(\beta)\Omega_0$ after the first N terms of its asymptotic series have been subtracted. Since $P(\beta)$ is given as an integral of the resolvent, we need only establish a strong asymptotic condition for $(H(\beta) - E)^{-1}\Omega_0$ with bounds uniform for $|E - E_0| = \varepsilon$. The remainder term we have to bound is just the remainder term of a geometric series:

$$[H(\beta) - E]^{-1}\Omega_0 - \sum_{n=0}^{N} (-\beta)^n (H_0 - E)^{-1}[V(H_0 - E)^{-1}]^n \Omega_0$$

$$= (-\beta)^{N+1}(H(\beta) - E)^{-1}[V(H_0 - E)^{-1}]^{N+1}\Omega_0$$

Since $\|(H(\beta) - E)^{-1}\|$ is uniformly bounded by the norm convergence we proved in the preceding section, we need only prove

$$\|[x^4(p^2 + x^2 - E)^{-1}]^{N+1}\Omega_0\| \leq C\sigma^{N+1}(N+1)!$$

for $|E - \frac{1}{2}| = \frac{1}{2}$. In terms of the standard A, $A^\dagger$ operators discussed in the appendix to Section V.3, $x^4 = \frac{1}{4}(A + A^\dagger)^4$ so that the norm in question can be bounded by $(2^4)^{N+1}$ terms of the form

$$4^{-N-1}\|A_1^\# \cdots A_4^\# (H_0 - E)^{-1} A_5^\# \cdots A_{4N+4}^\# (H_0 - E)^{-1}\Omega_0\|$$

where each $A^\#$ is either A or $A^\dagger$. The bound $C\sigma^{N+1}(N+1)!$ is proven by using the formulas

$$A\Omega_n = \sqrt{n}\,\Omega_{n-1}$$

$$A^\dagger\Omega_n = \sqrt{n+1}\,\Omega_{n+1}$$

$$(H_0 - E)^{-1}\Omega_n = (2n + 1 - E)^{-1}\Omega_n.$$

Therefore, the energy levels of a $p^2 + x^2 + \beta x^4$ oscillator obey a strong asymptotic condition; in particular, the energy levels of the anharmonic oscillator are determined uniquely by the Rayleigh–Schrödinger series.

Generalizations of the above argument to an abstract setting have been made by Simon. Typical of the results obtained is:

Theorem XII.20 Let H_0, V, and M be self-adjoint operators obeying:

(i) $H_0 \geq 0$.

(ii) For each $a > 0$, there is a b so that $V_- \leq aH_0 + b$.

(iii) For some c and d

$$|V| \leq cH_0^2 + d$$

(iv) $0 \leq M \leq H_0$.

(v) M and H_0 commute.

(vi) $C^\infty(M) \subset D(V)$ and V takes $C^\infty(M)$ into itself.

(vii) There are constants e and f so that for all n and all $\psi \in C^\infty(M)$,

$$\|(M+1)^n V\psi\| \leq e\|(M+f)^{n+2}\psi\|$$

Let $H_0 + \beta V$ be defined as a sum of forms for $|\beta|$ small, $|\arg \beta| < \pi - \varepsilon$. Then, for any isolated nondegenerate eigenvalue of H_0 there is an eigenvalue of $H_0 + \beta V$ for $|\beta|$ small that has the Rayleigh–Schrödinger series as strong asymptotic series.

For a proof, see the reference discussed in the Notes.

This theorem allows one to extend the idea of Example 1 to n-dimensional anharmonic oscillators. Specifically, if $\mathscr{H} = L^2(\mathbb{R}^n)$,

$$H_0 = \sum_{i=1}^{n} -\frac{\partial^2}{\partial x_i^2} + \omega_i^2 x_i^2$$

and

$$V = \sum_{i,j,k,\ell=1}^{n} a_{ijk\ell}\, x_i\, x_j\, x_k\, x_\ell$$

where a is such that $V(x) \geq 0$ for all $x \in \mathbb{R}^n$, then for any nondegenerate eigenvalue E_0 of H_0, the Rayleigh–Schrödinger series is a strong asymptotic series for the eigenvalue $E(\beta)$ of $H(\beta) = H_0 + \beta V$ with $E(0) = E_0$.

Example 2 ($(\varphi^4)_2$, spatially cut-off) In Section X.7, we briefly discussed spatially cut-off field theories in two-dimensional space time.

$$H_0 = \int \sqrt{m^2 + k^2}\, a^\dagger(k) a(k)\, dk = d\Gamma(\sqrt{k^2 + m^2})$$

$$V = \int g(x) {:}\varphi^4(x){:}\, dx$$

with $g \in L^2 \cap L^1$, $g \geq 0$, and

$$M = \int a^\dagger(k)a(k)\,dk = d\Gamma(1)$$

the number operator. All the conditions of Theorem XII.20 can be verified. The hardest condition to prove is (ii), which we discussed in Section X.9. Therefore, the Rayleigh–Schrödinger series for the ground state energy is a strong asymptotic series for the exact ground state energy. As we have already mentioned, the Rayleigh–Schrödinger series in this case is given by sums of Feynman diagrams. This example suggests that in more general circumstances the Feynman series might be a strong asymptotic series.

The strong asymptotic condition implies that $|a_n| \leq C\sigma^n n!$. There are series associated with simple examples for which a_n behaves like $(kn)!$ with $k > 1$. Thus, a strong asymptotic condition cannot hold in such cases. But a simple scaling argument and Carleman's theorem imply that any function g, analytic in the many-sheeted region $\{z \,|\, 0 < |z| < B;\ |\arg z| < \frac{1}{2}k\pi + \varepsilon\}$ with $|g(z)| \leq C\sigma^N[k(N+1)]!\,|z|^{N+1}$ for all N and z in the region, is identically zero. This suggests that we define:

Definition We say that a function $E(\beta)$, analytic in a sectorial region $\{\beta \,|\, 0 < |\beta| < B;\ |\arg \beta| < \frac{1}{2}k\pi + \varepsilon\}$, obeys a **modified strong asymptotic condition of order k** and has $\sum_{n=0}^{\infty} a_n \beta^n$ as an **order k strong asymptotic series** if there exist C and σ so that

$$\left| E(\beta) - \sum_{n=0}^{N} a_n \beta^n \right| \leq C\sigma^{N+1}[k(N+1)]!\,|\beta|^{N+1}$$

for all N and all β in the sector.

Because of the extension of Carleman's theorem, Theorem XII.19 extends: If f and g both have $\sum_{n=0}^{\infty} a_n \beta^n$ as order k strong asymptotic series, then $f = g$.

Example 3 (x^{2m} oscillator) Let $H_0 = -d^2/dx^2 + x^2$ and $V = x^{2m}$ $(m \geq 3)$. There is strong numerical evidence that the Rayleigh–Schrödinger coefficients a_n for the ground state energy behave as $(-1)^{n+1} C\sigma^n[(m-1)n]![1 + O(1/n)]$ for n large, which would imply that an ordinary strong asymptotic condition cannot hold. However, one can show that $E(\beta)$ has a continuation to a multisheeted sector $\{\beta \,|\, |\arg \beta| \leq \frac{1}{2}(m+1)\pi - \varepsilon;\ |\beta| \leq B_\varepsilon\}$ for any $\varepsilon > 0$ and that a strong asymptotic

condition of order $m-1$ holds in such a sector. Thus, the asymptotic series determines the eigenvalues in these cases also.

Since a strong asymptotic series determines $E(\beta)$ uniquely, one might expect there is a way of constructing E from the a_n and the knowledge that E obeys a strong asymptotic condition. The content of the following theorem of Watson, whose proof can be found in the references, is a method of constructing E explicitly:

Theorem XII.21 (Watson's theorem) Suppose that $E(\beta)$ has $\sum_{n=0}^{\infty} a_n \beta^n$ as strong asymptotic series in $\{\beta \mid 0 < |\beta| < B;\ |\arg \beta| \leq \frac{1}{2}\pi + \varepsilon\}$. Form the function

$$g(z) = \sum_{n=0}^{\infty} \frac{a_n}{n!} z^n$$

which is analytic in some circle about $z = 0$ because of the strong asymptotic condition. Then:

(a) g has an analytic continuation to the region $\{z \mid |\arg z| < \varepsilon\}$.
(b) If $|\beta| < B$ and $|\arg \beta| < \varepsilon$, then $\int_0^\infty |g(x\beta)| e^{-x}\, dx < \infty$.
(c) If $|\beta| < B$ and $|\arg \beta| < \varepsilon$, then $E(\beta) = \int_0^\infty g(x\beta) e^{-x}\, dx$.

Notice that since $\int_0^\infty x^n e^{-x}\, dx = n!$, if we could interchange $\int_0^\infty$ and $\sum_{n=0}^{\infty}$, we would have

$$\int_0^\infty g(x\beta) e^{-x}\, dx = \sum_{n=0}^{\infty} a_n \beta^n \qquad \text{(formally)}$$

The method we describe here for obtaining a sum for $\sum_{n=0}^{\infty} a_n \beta^n$ is a particular example of a **summability method**, that is, a method of obtaining a finite answer from a divergent series that is *formally* a sum for the series. This method is known as the **Borel summability method**; $g(z)$ is called the **Borel transform** of $\{a_n\}_{n=0}^{\infty}$; and the Laplace transform formula $\int_0^\infty g(x\beta) e^{-x}\, dx$ is sometimes called the inverse Borel transform.

Example 1, revisited We can take ε arbitrarily close to π so g is analytic in the cut plane $\mathbb{C} \backslash (-\infty, -R)$, where R is the radius of convergence of the Borel transform. In the special case of a one-dimensional oscillator, it is known that $E(\beta)$ is analytic in $\{\beta \mid |\arg \beta| < \pi\}$, so the inverse Borel transform converges to E for any positive β (and more generally for any β with $\operatorname{Re} \beta > 0$).

Example 2, revisited In this case, we can recover $E(\beta)$ for $|\beta|$ and $|\arg \beta|$ sufficiently small from the Borel transform for the Rayleigh–Schrödinger series.

Example 3, revisited The Borel method is not directly applicable, but a generalization works (Problem 29(b)). Explicitly, for the x^{2m} oscillator, the modified Borel transform

$$g(z) = \sum_{n=0}^{\infty} \frac{a_n}{[n(m-1)]!} z^n$$

is analytic in the cut plane $\mathbb{C}\backslash(-\infty, -R_m)$ and for β positive and small,

$$E(\beta) = \int_0^{\infty} g(\beta x^{m-1}) e^{-x}\, dx$$

We have just seen that a particular summability method can be used to recover the eigenvalues. In certain special cases, other methods that are often computationally more convenient have been shown to work; we discuss them briefly in the Notes.

XII.5 Spectral concentration

In the preceding two sections we analyzed perturbed systems that have an isolated eigenvalue near an isolated unperturbed eigenvalue and a perturbation series that is finite order by order but that does not converge. In this section we wish to consider the more complex situation where there is an isolated unperturbed eigenvalue and a perturbation series that is finite term by term but where there is no perturbed eigenvalue!

Consider the following simple example: Let $H_0 = -\Delta - 1/r$ and let $V = E_0\, \mathbf{e} \cdot \mathbf{r}$ where $\mathbf{e}$ is a fixed unit vector in $\mathbb{R}^3$. For β real, $H_0 + \beta V$ is the Hamiltonian of a hydrogen atom in a constant electric field $-\beta E_0\, \mathbf{e}$, the so-called Stark effect Hamiltonian. In Section X.5 we proved that $H_0 + \beta V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. On the other hand, it is easy to see that if $\beta \neq 0$, $H_0 + \beta V$ is not bounded below. We will show (Section XIII.4) that $\sigma(H_0 + \beta V) = (-\infty, \infty)$ if $\beta \neq 0$. Thus, as soon as the perturbation is turned on, all the eigenvalues of H_0 are drowned in the continuous spectrum. Nevertheless, the perturbation series for the ground state energy, given by the formal expressions in Section 1, is finite term by term. What does it mean?

Before presenting the mathematical resolution of this question, let us consider an alternative interpretation. Let

$$V_n(r) = \begin{cases} E_0\,\mathbf{e}\cdot\mathbf{r} & \text{if} \quad |\mathbf{e}\cdot\mathbf{r}| < n \\ E_0 n & \text{if} \quad \mathbf{e}\cdot\mathbf{r} \geq n \\ -E_0 n & \text{if} \quad \mathbf{e}\cdot\mathbf{r} \leq -n \end{cases}$$

Each V_n is a perturbation of type (A) so, for some $B^{(n)}$, the perturbation series $\sum a_m^{(n)}\beta^m$ for the ground state energy $E^{(n)}(\beta)$ of $H_0 + \beta V_n$ converges to $E^{(n)}(\beta)$ if $|\beta| \leq B^{(n)}$. Suppose that $\sum_{m=0}^{\infty} a_m \beta^m$ is the formal perturbation series for the ground state energy of $H_0 + \beta V$. We notice that $a_m^{(n)}$ converges to a_m as $n \to \infty$. We thus interpret $\sum_{m=0}^{\infty} a_m \beta^m$ as a formal limit of the convergent series $\sum_{m=0}^{\infty} a_m^{(n)}\beta^m$. This interpretation is not very satisfying mathematically for it is likely that $B^{(n)} \to 0$ and that $\sum_{m=0}^{\infty} a_m \beta^m$ diverges for all β, but it must be emphasized that it is the right physical interpretation! For experiments done on real atoms in real fields are not done with an electric field extending through all of space—the potential V is an idealization. V_n is much closer to the experimentally obtained potential and $E^{(n)}(\beta)$ to the measured spectroscopic observables. But since $E^{(n)}(\beta) \simeq a_0 + a_1^{(n)}\beta$ for β small and $a_1^{(n)} \simeq a_1$ for n large, we can estimate $E^{(n)}(\beta)$ using a_1.

In spite of the above remark on physical relevance, one cannot help feeling that the perturbation series has something to do with $H_0 + \beta V$. What we shall see is that the spectrum of $H_0 + \beta V$ "bunches up" near the unperturbed eigenvalue and that the center of this spectral concentration is given by an asymptotic series $\sum a_m \beta^m$. The exact meaning of this notion of "bunching up" is given by:

Definition Let H_n be a family of self-adjoint operators and let $\{P_n(\Omega)\}$ be the family of spectral projections of H_n. Let $\{S_n\}_{n=1}^{\infty}$ and T be subsets of $\mathbb{R}$. We say **the part of the spectrum of H_n in T is asymptotically in S_n** if and only if

$$\text{s-}\lim_{n\to\infty} P_n(T\backslash S_n) = 0$$

If $H_n \to H$ in strong resolvent sense, we say **the part of the spectrum of H_n in S_n is asymptotically the part of the spectrum of H in T** if

$$\text{s-}\lim_{n\to\infty} P_n(S_n) = P(T)$$

where $\{P(\Omega)\}$ is the projection-valued measure of H.

Example 1 Let $H = I$, $H_n = I + n^{-1}X$ where X is the operator $(Xf)(x) = xf(x)$ on $L^2(-\infty, \infty)$. If $\chi_{(a,b)}$ is multiplication by the characteristic function of (a, b), then $P_n(1-\alpha, 1+\beta) = \chi_{(-n\alpha, n\beta)}$. In particular, the part of the spectrum of H_n in $(0, 2)$ is asymptotically in $(1 - n^{-1/2}, 1 + n^{-1/2})$, and the part of the spectrum of H_n in $(1 - n^{-1/2}, 1 + n^{-1/2})$ is asymptotically the part of the spectrum of H in $(0, 2)$. To see the connection between this asymptotic containment and the intuitive notion of "bunching up," consider the spectral measures associated with a fixed vector ψ. If $d\mu_n(\lambda) = d(\psi, P_n(\lambda)\psi)$, then $d\mu_n(\lambda) = d\mu_1(1 + (\lambda - 1)n^{-1})$. Thus $d\mu_n \to \delta(\lambda - 1)$.

In this example, we observe a characteristic symmetry:

Proposition Suppose that $H_n \to H$ in strong resolvent sense. Let $T = (a, b)$ with $a, b \notin \sigma_{pp}(H)$. Let $S_n \subset T$ for n sufficiently large. Then the part of the spectrum of H_n in T is asymptotically in S_n if and only if the part of the spectrum of H_n in S_n is asymptotically the part of the spectrum of H in T.

Proof By Theorem VIII.24, s-lim $P_n(T) = P(T)$. Thus s-lim $P_n(S_n) = P(T)$ if and only if s-lim $P_n(T \setminus S_n) = 0$. ∎

We also emphasize that the notion of asymptotic concentration is a property of a *sequence* of operators $\{H_n\}_{n=1}^{\infty}$. It makes no sense to say that a single operator H_n has spectrum concentrated in S_n. In Example 1 all the H_n are unitarily equivalent, so $\sigma(H_n) = \sigma(H_m)$.

We can now make a conjecture about the relation of $a_0 + a_1\beta$ to $H_0 + \beta V$ in our Stark effect example. Suppose that we can find an interval I about the unperturbed ground state energy a_0 with $\sigma(H_0) \cap I = \{a_0\}$ and a function $f(\beta)$ with $f(\beta)/\beta \to 0$ so that the part of the spectrum of $H(\beta)$ in $(a_0 + a_1\beta - f(\beta), a_0 + a_1\beta + f(\beta))$ is asymptotically the part of spectrum of H_0 in I. This property determines a_1 uniquely (Problem 31). Thus, while $H(\beta)$ does not have an eigenvalue near $a_0 + \beta a_1$, it does have spectrum concentrated near $a_0 + \beta a_1$ as $\beta \to 0$. Our tool for proving this spectral concentration is the notion of pseudo-eigenvalue:

Definition Suppose that $H(\beta)$ is a family of self-adjoint operators defined for β real and small so that $H(\beta) \to H_0$ as $\beta \to 0$ in strong resolvent sense. Let E_0 be an isolated nondegenerate eigenvalue of H_0 and ψ_0 be the corresponding normalized eigenvector. A family of vectors $\psi(\beta)$, β real, and numbers

$E_0 + \beta E_1$ are called a **first order pseudo-eigenvector** and a **first order pseudo-eigenvalue** respectively if and only if:

(i) $\lim_{\beta \to 0} \|\psi(\beta) - \psi_0\| = 0$;
(ii) $\lim_{\beta \to 0} \beta^{-1} \|(H(\beta) - E_0 - \beta E_1)\psi(\beta)\| = 0$.

The statement "$E_0 + \beta E_1$ is a first order pseudo-eigenvalue of $H(\beta)$" will be used as a shorthand for the statement that there exists a first order pseudo-eigenvector $\psi(\beta)$ with $E_0 + \beta E_1$ the associated pseudo-eigenvalue.

Theorem XII.22 Suppose that $H(\beta) \to H_0$ in strong resolvent sense as $\beta \to 0$ with all the $H(\beta)$ self-adjoint. Let E_0 be an isolated nondegenerate eigenvalue of H_0 and I an interval so that $\bar{I} \cap \sigma(H_0) = \{E_0\}$. Then there exists a function $f(\beta)$, obeying $f(\beta)/\beta \to 0$, so that the part of the spectrum of $H(\beta)$ in I is asymptotically in

$$I_\beta \equiv (E_0 + \beta E_1 - f(\beta), E_0 + \beta E_1 + f(\beta))$$

if and only if $E_0 + \beta E_1$ is a first order pseudo-eigenvalue for $H(\beta)$.

Proof Let $P^\beta(\Omega)$ be the spectral projections of $H(\beta)$. If the part of $\sigma(H(\beta))$ in I is asymptotically in I_β, then $P^\beta(I_\beta)$ converges strongly to $P^0(I) = P^0(\{E_0\})$. In particular, if ψ_0 is the unperturbed eigenvector for H and $\psi(\beta) = P^\beta(I_\beta)\psi_0$, then $\psi(\beta) \to \psi_0$ in norm. Moreover,

$$\beta^{-1}\|[H(\beta) - E_0 - E_1\beta]\psi(\beta)\| \leq \beta^{-1} f(\beta)\|\psi(\beta)\| \to 0$$

as $\beta \to 0$, so $E_0 + E_1\beta$ is a first order pseudo-eigenvalue.

Conversely, suppose that $E_0 + \beta E_1$ is a pseudo-eigenvalue with $\psi(\beta)$ as pseudo-eigenvector. Let

$$f(\beta) = \|[H(\beta) - E_0 - E_1\beta]\psi(\beta)\|^{1/2}\beta^{1/2}$$

Then $\beta^{-1} f(\beta) \to 0$ as $\beta \to 0$. We shall show that $P^\beta(I_\beta)$ converges to $P^0(\{E_0\})$ strongly.

$$\begin{aligned}
\beta^{-2} f(\beta)^4 &= \|[H(\beta) - E_0 - E_1\beta]\psi(\beta)\|^2 \\
&= \int_{-\infty}^{\infty} (\lambda - E_0 - E_1\beta)^2 \, d(\psi(\beta), P^\beta(\lambda)\psi(\beta)) \\
&\geq f(\beta)^2 \int_{\lambda \notin I_\beta} d(\psi(\beta), P^\beta(\lambda)\psi(\beta)) \\
&= f(\beta)^2 \|(I - P^\beta(I_\beta))\psi(\beta)\|^2
\end{aligned}$$

Thus $\|(I - P^\beta(I_\beta))\psi(\beta)\| \leq \beta^{-1} f(\beta) \to 0$. Since

$$\|(I - P^\beta(I_\beta))\psi_0\| \leq \|(I - P^\beta(I_\beta))\psi(\beta)\| + \|\psi(\beta) - \psi_0\|$$

we conclude that

$$(I - P^\beta(I_\beta))P^0(\{E_0\}) \to 0$$

in norm. Therefore,

$$P^\beta(I \backslash I_\beta)P^0(\{E_0\}) = P^\beta(I \backslash I_\beta)(1 - P^\beta(I_\beta))P^0(\{E_0\}) \to 0$$

In addition, the strong resolvent convergence implies that $P^\beta(I) \to P^0(\{E_0\})$, and thus that

$$P^\beta(I \backslash I_\beta)(1 - P^0(\{E_0\})) \xrightarrow{s} 0$$

We conclude that $P^\beta(I \backslash I_\beta) \xrightarrow{s} 0$. ∎

Theorem XII.23 Suppose that self-adjoint operators $H(\beta)$ are given for each β in some neighborhood N of $0 \in \mathbb{R}$. Let $H_0 \equiv H(0)$ and suppose that there is a symmetric operator V such that:

(i) H_0 is essentially self-adjoint on $D(H_0) \cap D(V)$.
(ii) If $\varphi \in D(H_0) \cap D(V)$, then for any $\beta \in N$, we have that $\varphi \in D(H(\beta))$ and $H(\beta)\varphi = H_0\varphi + \beta V\varphi$.
(iii) E_0 is an isolated eigenvalue of H_0 of multiplicity 1 and the associated eigenvector ψ_0 is in $D(V)$.

Let I be an open interval with $\sigma(H_0) \cap \bar{I} = \{E_0\}$ and let $E_1 = (\psi_0, V\psi_0)$ be the first-order Rayleigh–Schrödinger coefficient for the perturbation of the eigenvalue E_0.

Then, there is a function $f(\beta)$ with $\beta^{-1} f(\beta) \to 0$ so that the part of the spectrum of $H_0 + \beta V$ in I is asymptotically in $(E_0 + E_1\beta - f(\beta), E_0 + E_1\beta + f(\beta))$.

Proof A simple argument using (i), (ii) and the first resolvent equation proves that $H(\beta) \to H_0$ in strong resolvent sense as $\beta \to 0$ (Problem 32). By Theorem XII.22, it is sufficient to construct a first order pseudo-eigenvector $\psi(\beta)$ with pseudo-eigenvalue $E_0 + E_1\beta$. Let $\{P^\beta(\Omega)\}$ be the spectral projections for $H(\beta)$. Choose $\psi(\beta) = P^\beta(I)\psi_0$. By Theorem VIII.24, s-lim $P^\beta(I) =$

$P^0(I)$, so $\psi(\beta) \to \psi_0$ as $\beta \to 0$. Since $\psi_0 \in D(H(\beta))$ for any $\beta \in N$, $P^\beta(I)H(\beta)\psi_0 = H(\beta)P^\beta(I)\psi_0$. Thus

$$\begin{aligned}\|\beta^{-1}(H(\beta) - E_0 - \beta E_1)\psi(\beta)\| &= \|\beta^{-1}P^\beta(I)(H_0 + \beta V - E_0 - E_1\beta)\psi_0\| \\ &= \|P^\beta(I)(V - E_1)\psi_0\| \\ &\le \|[P^\beta(I) - P^{(0)}(I)](V - E_1)\psi_0\| \\ &\quad + \|P^{(0)}(I)(V - E_1)\psi_0\|\end{aligned}$$

Since s-lim $P^\beta(I) = P^{(0)}(I)$, the first term in the final expression converges to 0. Since E_0 is nondegenerate, $P^{(0)}(I)\varphi = (\psi_0, \varphi)\psi_0$ and thus

$$P^0(I)(V\psi_0) = E_1\psi_0$$

Therefore the second term in the final expression is 0. This proves that $\psi(\beta)$ is a first-order pseudo-eigenvector. ∎

Example 2 (Stark effect for the hydrogen atom) Let $H_0 = -\Delta - 1/r$ and let $V = E_0\,\mathbf{e}\cdot\mathbf{r}$. Then $E_0 = -\frac{1}{4}$ is the ground state energy of H_0. By Theorem X.38, $H_0 + \beta V$ is essentially self-adjoint on $D(H_0) \cap D(V)$. Moreover, ψ_0 is known explicitly and $|\psi_0(x)| \le C\exp(-|x|/2)$ for suitable C. In particular, $\psi_0 \in D(V)$. Thus, the hypotheses of Theorem XII.23 are satisfied. Since $E_1 \equiv (\psi_0, V\psi_0) = 0$, we conclude that, as $\beta \to 0$, the part of the spectrum of $H_0 + \beta V$ near E_0 is concentrated in $(E_0 - \lambda\beta, E_0 + \lambda\beta)$ for any $\lambda > 0$. In addition one can prove that all the coefficients of the Rayleigh–Schrödinger series are finite. Moreover, for any n, one can find $f^{(n)}(\beta)$ with $|\beta|^{-n}f^{(n)}(\beta) \to 0$ so that the part of the spectrum of $H_0 + \beta V$ near E_0 is concentrated in $(\sum_{m=0}^n E_m\beta^m - f^{(n)}(\beta),\ \sum_{m=0}^n E_m\beta^m + f^{(n)}(\beta))$ as $|\beta| \to 0$.

In addition to the generalization to order n mentioned in the preceding example, Theorem XII.23 has another important generalization: Discrete levels of finite but nontrivial degeneracy can be treated. For instance, in the Stark effect example above, the first eigenvalue above the ground state is fourfold degenerate and splits into one two-dimensional pseudo-eigenvalue and two one-dimensional pseudo-eigenvalues to first order. Explicitly, one can find four linearly independent first-order pseudo-eigenvectors converging to vectors ψ_i satisfying $H_0\psi_i = -\frac{1}{16}\psi_i$ and with pseudo-eigenvalues, $-\frac{1}{16}$ twice and $-\frac{1}{16} \pm a\beta$, where a can be computed using "degenerate perturbation theory."

XII.6 Resonances and the Fermi golden rule

Whenever calculus is brought in, or higher algebra, you could take it as a warning signal that the operator was trying to substitute theory for experience.

B. Graham, The Intelligent Investor

Thus far we have been considering successively more singular perturbations of isolated eigenvalues. In Section 2 we considered the case where a perturbed eigenvalue and a convergent perturbation series exist, and in Sections 3 and 4 the case where a perturbed eigenvalue exists but the associated perturbation series is divergent. In the examples of Section 5, there is not even a perturbed eigenvalue. In this section we consider a still more singular, although, as we shall see, physically relevant, case where it is not only true that there is no perturbed eigenvalue but where the unperturbed eigenvalue is not isolated.

A simple example of this phenomenon occurs if

$$H_0 = -\Delta_1 - \frac{2}{r_1} - \Delta_2 - \frac{2}{r_2}$$

and $V = |\mathbf{r}_1 - \mathbf{r}_2|^{-1}$ on $L^2(\mathbb{R}^6)$. We will write points of $\mathbb{R}^6$ as $\langle \mathbf{r}_1, \mathbf{r}_2 \rangle$ with $\mathbf{r}_i \in \mathbb{R}^3$. $H_0 + V$ is the Hamiltonian of the helium atom if we ignore relativistic corrections and go to the limit of infinite nuclear mass. If $h = -\Delta - 2/r$ on $L^2(\mathbb{R}^3)$, then $H_0 = 1 \otimes h + h \otimes 1$. Since h and H_0 are self-adjoint, we can use Theorem VIII.33 to compute the spectrum of H_0 in terms of the spectrum of h under the natural identification of $L^2(\mathbb{R}^6)$ with $L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$. The eigenvalues of h are explicitly known to be $\{-1/n^2\}_{n=1}^{\infty}$, so H_0 has eigenvalues

$$\{E_{n,m}\} \equiv \left\{-\left(\frac{1}{n^2} + \frac{1}{m^2}\right)\right\}_{n,m=1}^{\infty}$$

Moreover, $\sigma_{\text{ess}}(h) = [0, \infty)$, so $\sigma_{\text{ess}}(H_0) = [-1, \infty)$. Thus

$$\sigma(H_0) = \{x + y \,|\, x, y \in [0, \infty) \cup \{-1/n^2\}_{n=1}^{\infty}\}$$

$$= \left\{-1 - \frac{1}{n^2}\right\}_{n=1}^{\infty} \cup [-1, \infty)$$

Therefore, the eigenvalues $E_{n,m}$ are in the continuous spectrum if $n \geq 2$ and $m \geq 2$. See Figure XII.2. When the perturbation V is turned on, one expects from physical considerations that the eigenvalues in the continuous spectrum will "dissolve." This expectation is correct except for two qualifications

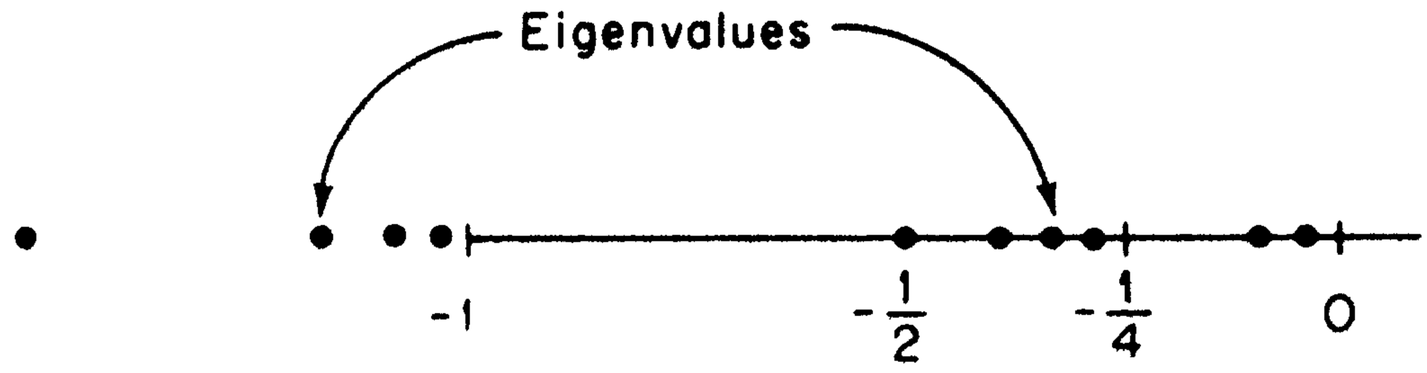


FIGURE XII.2 The spectrum of H_0.

discussed in the Notes. However, one observes a "memory" of these eigenvalues of H_0 in the physics of the helium atom. In the scattering of electrons off helium ions, one observes bumps in the scattering cross section for total $He^+ + e$ energies near the energies $E_{n,m}$ (in practice, only the bumps for small m and n can be distinguished from "background"). See Figure XII.3. Similar bumps are found in the absorption of light by helium, i.e., at frequencies of incident light for which the energy of a light quantum is

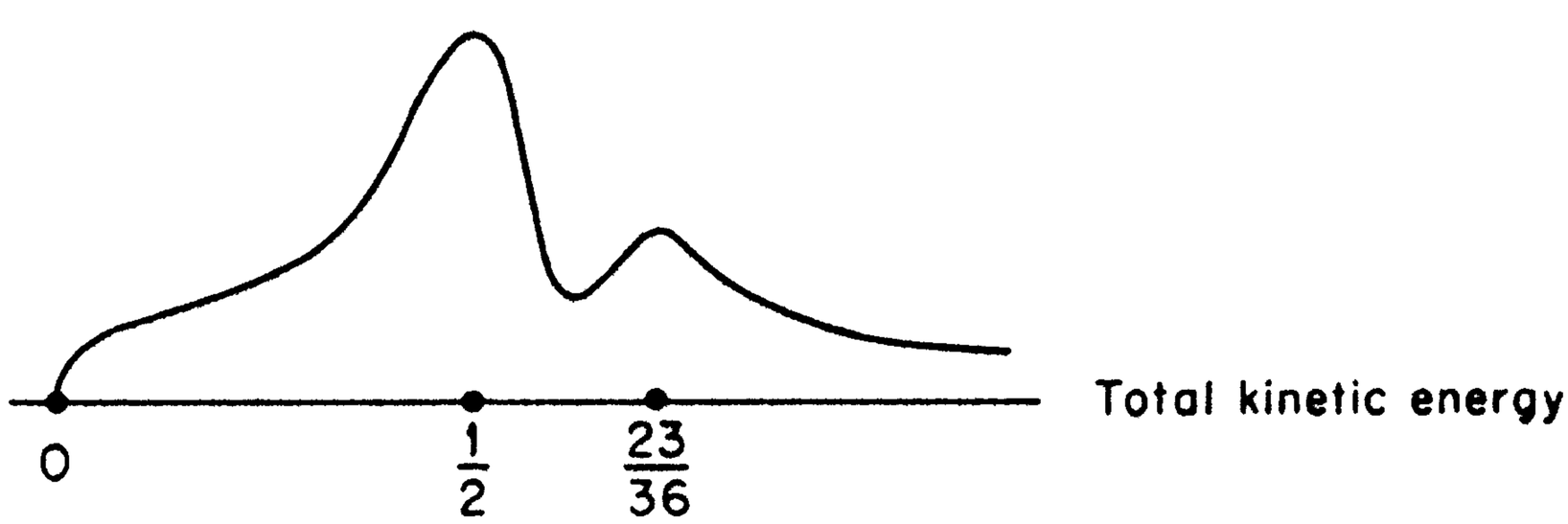


FIGURE XII.3 Schematic elastic scattering cross section for $e + He^+ \rightarrow e + He^+$.

near the difference of $E_{n,m}$ and $E_{1,1}$ (= ground state energy) light is absorbed strongly (Figure XII.4). We emphasize that our diagrams for scattering and absorption are schematic. Specifically, the energies $E_{n,m}$ are shifted due to the perturbation V.

Not only are these bumps, called **Auger** or **autoionizing** states, observed, but their widths are fairly well described by a calculational method known as Fermi's golden rule which has a purely heuristic derivation which we describe in the Notes. The derivation is based on a physical model for the mechanism that produces the bumps. In the remainder of this section we first isolate the mathematical quantity corresponding to the widths of the bumps and then show how the Fermi golden rule is a consequence of the

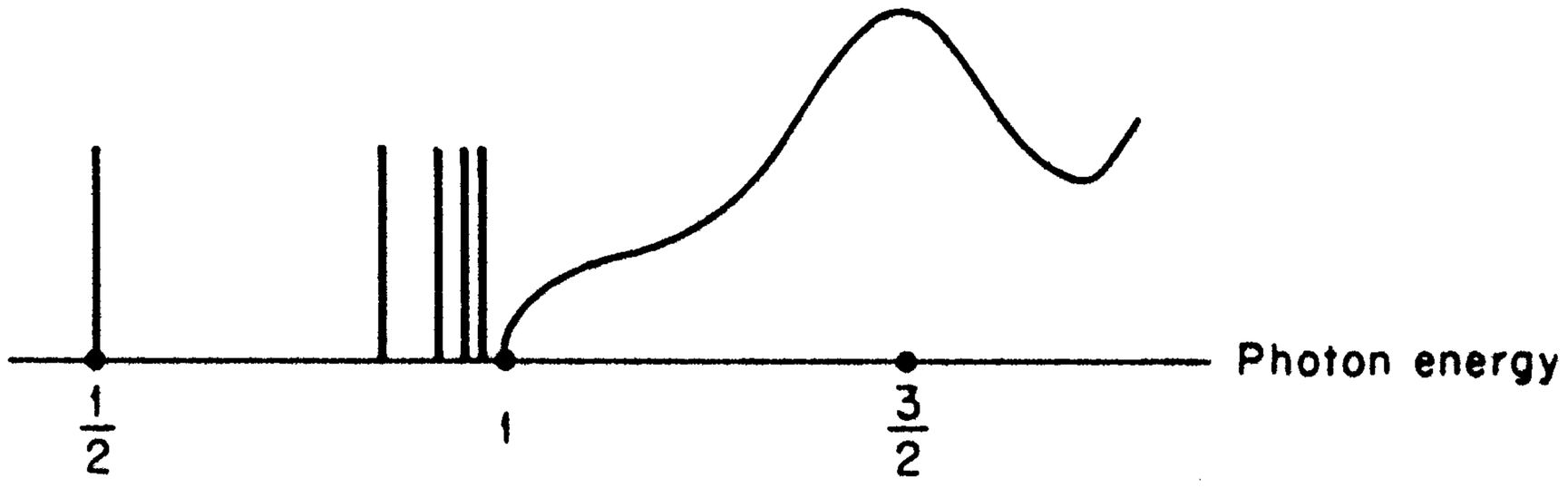


FIGURE XII.4 Schematic absorption cross section for $He + \gamma$.

Kato–Rellich theory of regular perturbations, at least in this helium atom situation. We emphasize that the Fermi golden rule has been applied successfully to many physical situations where it has not yet been rigorously justified.

Our interpretation of the Fermi golden rule will be in three steps, two of them "quasi-mathematical" and the last rigorous mathematics. The goal of the first two steps will be to isolate a quantity susceptible to exact mathematical analysis. While this quantity is not precisely the width of a bump, it will be related to the width by a set of nonrigorous arguments. This situation is not an uncommon one in mathematical physics: The mathematically precise quantities are not equal to experimental quantities but are related to them by some nonrigorous argument. There is thus an important element of extramathematical taste in certain problems of mathematical physics.

Our first step is to relate the width of bumps to the imaginary part of the position of poles of "the scattering amplitude." The second step is to look at poles in the analytic continuation of the resolvent. Thus the quasi-mathematical part of the analysis will be to replace the nonprecise "width of the bump" with the precise "imaginary part of the position of a pole on the second sheet of the analytic continuation of the expectation value of the resolvent on a dense set of states." Our study of this precise quantity will be accomplished by proving it equal to the imaginary part of an eigenvalue of a certain non-self-adjoint operator. The main technical device in this proof will be scaling techniques which we study further in Section XIII.10.

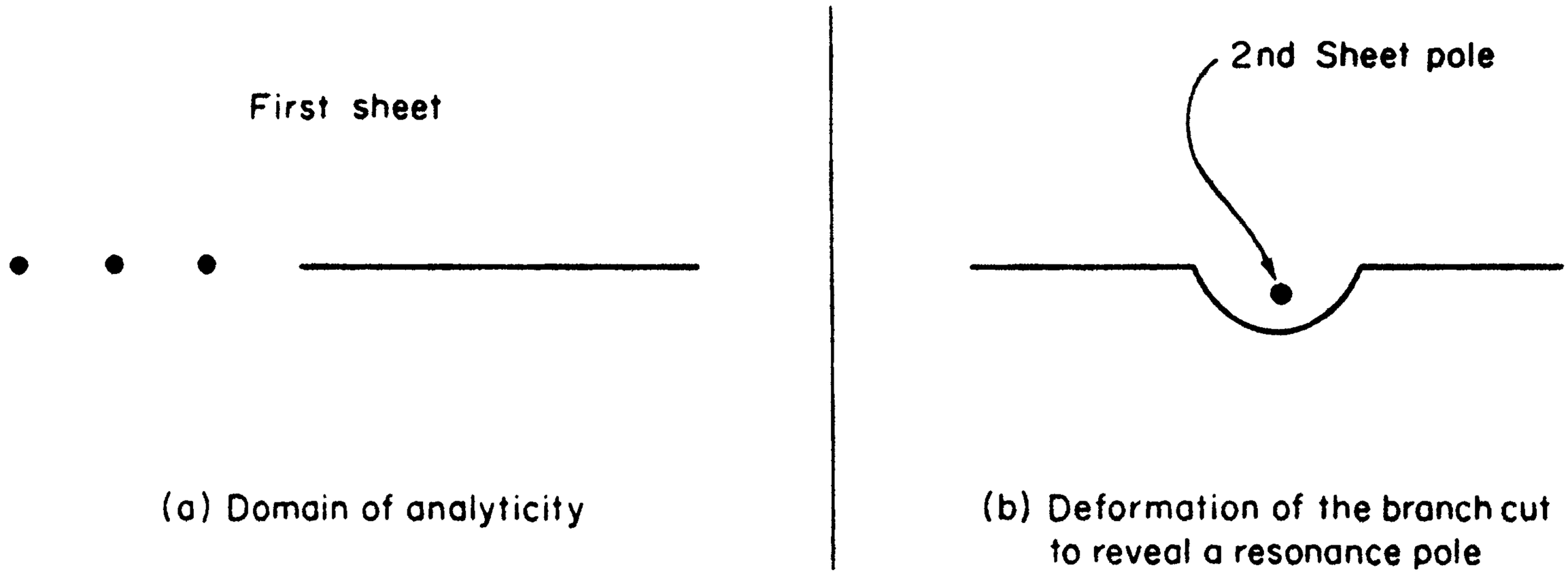
Scattering is described in quantum-mechanical situations as the square of the modulus of the "scattering amplitude" (see Section XI.6). The scattering amplitude, which is a complex-valued function of the energy and scattering angle, is typically an analytic function of energy (see Section XI.7) in a cut plane $\mathbb{C}\backslash\sigma(H)$, where H is the Hamiltonian of the interacting quantum system. Suppose that the scattering amplitude $f(E)$ has an analytic continuation onto a second sheet (Figure XII.5) and that there is a simple pole on the second sheet at a position $E_r - i\Gamma/2$ very near the real axis. Thus,

$$f(E) = \frac{C}{E - E_r + \frac{1}{2}i\Gamma} + f_b(E)$$

where the background f_b is analytic at $E = E_r - \frac{1}{2}i\Gamma$. If the pole is very near the real axis and if $f_b(E_r)$ is not too large, then

$$|f(E)|^2 = \frac{|C|^2}{(E - E_r)^2 + \frac{1}{4}\Gamma^2} + R$$

where the remainder R will be small near $E = E_r$. In Figure XII.6, we plot the **Breit–Wigner** resonance shape: $|C|^2((E - E_r)^2 + \frac{1}{4}\Gamma^2)^{-1}$. Notice that its



(a) Domain of analyticity

(b) Deformation of the branch cut to reveal a resonance pole

FIGURE XII.5 Continuation of the scattering amplitude.

width at half maximum is Γ. The pole in $f(E)$ is called a resonance pole and Γ is called the **width** of the resonance. If the pole term is much larger than the background term for $E = E_r$, Γ will approximate the width of a "bump" in $|f(E)|^2$. We have thus accomplished half of our quasi-mathematical task of "isolating" the width of a bump.

The second half of the task requires us to appeal to the fact that the scattering amplitude is related to boundary values of the resolvent $(H - E)^{-1}$ as E approaches the real axis from the upper half-plane (see Sections XI.6 and XI.7). For this reason, we seek a method of continuing $(\psi, (H - E)^{-1}\psi) = R_\psi(E)$ to the second sheet. If we find that such a continuation is possible for a dense set of $\psi \in \mathscr{H}$ and that for this dense set, the function $R_\psi(E)$ has a pole at $E = E_r - \frac{1}{2}i\Gamma$, we will associate E with a resonance pole, and Γ with a resonance width. Of course, we need a reason to think the pole is to be associated with H rather than the particular dense set of ψ, and so we shall consider only ψ for which $(\psi, (H_0 - z)^{-1}\psi)$ also has a continuation to the second sheet but without a pole at $E_r - \frac{1}{2}i\Gamma$.

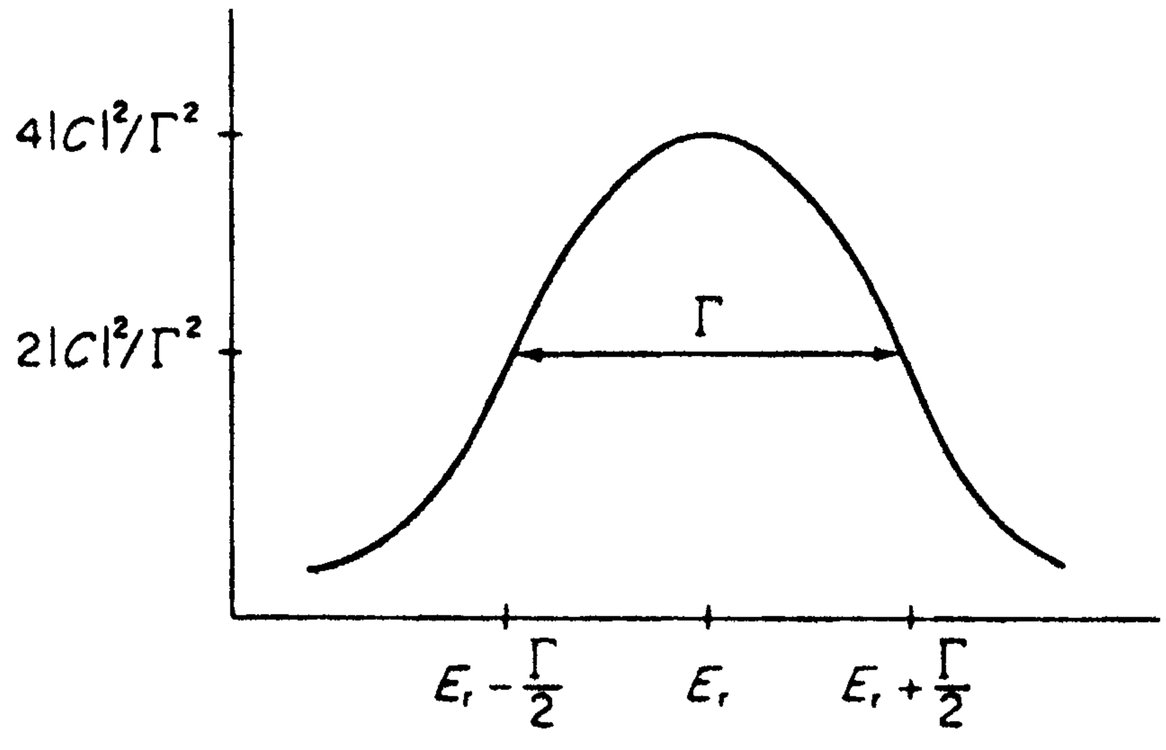


FIGURE XII.6 A Breit–Wigner resonance shape.

We have thus completed the task of finding a mathematical quantity to analyze:

Definition Suppose that there is a dense set of vectors $D \subset \mathscr{H}$ such that for all $\psi \in D$, both $(\psi, (H - z)^{-1}\psi) = R_\psi(z)$ and $(\psi, (H_0 - z)^{-1}\psi) = R_\psi^{(0)}(z)$ have analytic continuations onto the second sheet (across the real axis from the upper half-plane of the first sheet). If $R_\psi^{(0)}(z)$ is analytic at $z_0 = E_r - \frac{1}{2}i\Gamma$ and $R_\psi(z)$ has a pole at z_0 for some ψ, we say that z_0 is a **resonance pole**. Γ is called the **width** of the resonance.

We like to think of Γ as the width of a bump, but this step is not precise: First, the formula relating the scattering amplitude to the resolvent does not always involve expectation values of vectors $\psi \in D$; secondly, the "background" may not be negligible.

To study these resonance poles, we need the technical device of dilations. Here we just sketch the ideas involved and apply them to the operator $-\Delta - 2/r$ and the helium Hamiltonian. In Section XIII.10 we present a detailed development of dilation methods and apply them to a general class of operators. For θ real, we define $u(\theta)$ on $L^2(\mathbb{R}^3)$ by

$$(u(\theta)f)(r) = e^{3\theta/2}f(e^\theta r)$$

$u(\theta)$ is a one-parameter unitary group on $L^2(\mathbb{R}^3)$. It is easy to see that the $u(\theta)$ leave $D(h) = D(-\Delta)$ invariant and that

$$h(\theta) \equiv u(\theta)hu(\theta)^{-1} = -e^{-2\theta}\Delta - \frac{2e^{-\theta}}{r}$$

The first crucial fact, which follows from Theorems X.12 and XII.9, is that $h(\theta)$ has a continuation to a family of operators analytic in the sense of Kato in the whole plane.

Let us find the spectrum of $h(\theta)$. The spectrum of $-\Delta$ is $[0, \infty)$. By Theorem XIII.14 and the fact that $r^{-1}(-\Delta + 1)^{-1}$ is Hilbert–Schmidt, $-\Delta - 2e^\theta/r$ will have spectrum $[0, \infty)$ plus a possible set of isolated points outside of $[0, \infty)$ even when θ is nonreal. Moreover, each of the points outside $[0, \infty)$ is an eigenvalue of finite multiplicity. Thus $h(\theta)$ has spectrum $\{e^{-2\theta}\lambda \mid \lambda \in [0, \infty)\}$ plus some possible additional discrete spectrum. The points of the discrete spectrum will be given by analytic functions $f(\theta)$ of θ (with possible algebraic singularities) according to Theorems XII.8 and XII.13. But

$$u(\theta_0)h(\theta_1 + i\theta_2)u(\theta_0)^{-1} = h(\theta_1 + \theta_0 + i\theta_2)$$

for $\theta_1, \theta_2, \theta_0$ real. Thus $h(\theta_1 + i\theta_2)$ is unitarily equivalent to $h(\theta_1' + i\theta_2)$. As a consequence, they have the same eigenvalues. Therefore, the functions $f(\theta)$

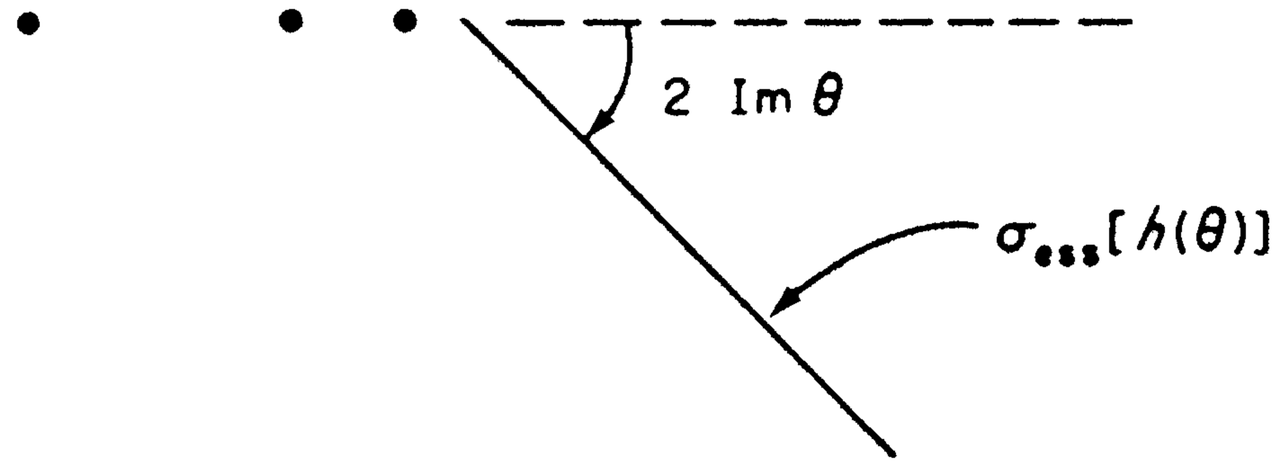


FIGURE XII.7 $\sigma(h(\theta))$, $0 \leq \operatorname{Im} \theta \leq \pi/2$.

are constant if Im θ is constant. Since the $f(\theta)$ are analytic, they are constant for all θ. For $\theta = 0$, $\sigma_{pp}(h) = \{-1/n^2\}_{n=1}^{\infty}$ so

$$\sigma(h(\theta)) = \{e^{-2\theta}\lambda \,|\, \lambda \in [0, \infty)\} \cup \{-1/n^2\}_{n=1}^{\infty}$$

(Figure XII.7). In the above we have not proven that $h(\theta)$ could not have eigenvalues in the sector $0 > \arg \lambda > -2 \operatorname{Im} \theta$, but a detailed analysis using the explicit solutions of the Coulombic–Schrödinger equation shows that they do not occur.

Next we consider scaling for H_0 and $H_0 + \beta V$. Define $U(\theta)$ on $\mathbb{R}^6$ by $(U(\theta)F)\ (\mathbf{r}_1, \mathbf{r}_2) = e^{3\theta}\ F(e^{\theta}\mathbf{r}_1, e^{\theta}\mathbf{r}_2)$, for θ real. Also for θ real, let $V(\theta) \equiv U(\theta)VU(\theta)^{-1} = e^{-\theta}V$ and $H_0(\theta) \equiv U(\theta)\ H_0\ U(\theta)^{-1} = h(\theta) \otimes 1 + 1 \otimes h(\theta)$. Both $H_0(\theta)$ and $V(\theta)$ have type (A) analytic continuations to the whole complex plane. For any θ, $H_0(\theta)$ is of the form $A \otimes 1 + 1 \otimes B$, although A and B are not self-adjoint. We shall prove that

$$\sigma(A \otimes 1 + 1 \otimes B) = \{x + y \,|\, x \in \sigma(A),\ y \in \sigma(B)\}$$

in Section XIII.9. Thus

$$\sigma(H_0(\theta)) = \{x + y \,|\, x,\ y \in \sigma(h_0(\theta))\} = \bigcup_{n=1}^{\infty} \left\{ -\frac{1}{n^2} + \lambda e^{-2\theta} \,\middle|\, \lambda \geq 0 \right\}$$

$$\cup \left\{ -\frac{1}{n^2} - \frac{1}{m^2} \,\middle|\, n, m \text{ integral} \right\} \cup \{\lambda e^{-2\theta} \,|\, \lambda \geq 0\}$$

(see Figure XII.8). In particular, the eigenvalues embedded in $\sigma(H_0)$ are isolated discrete eigenvalues of $H_0(\theta)$ for θ nonreal. The eigenvalues $E_{n,m}$

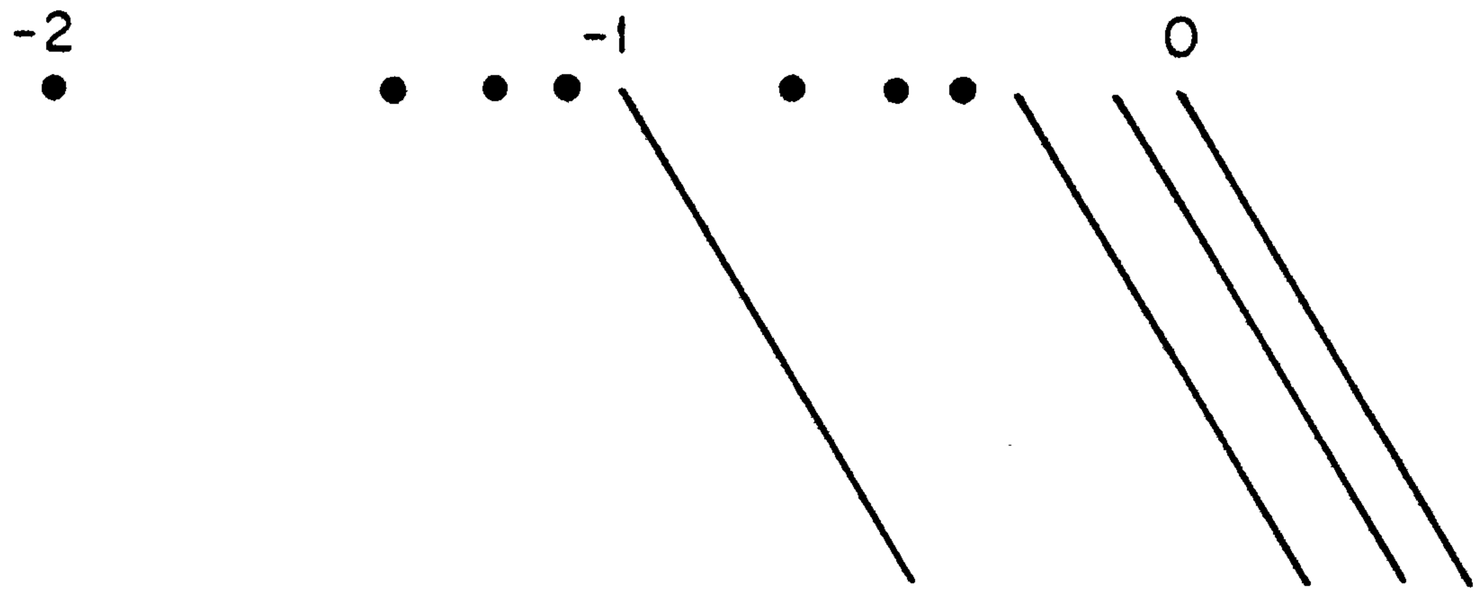


FIGURE XII.8 $\sigma(H_0(\theta))$.

$(n, m \geq 2)$ are all degenerate. It is possible to use symmetries to decompose $L^2(\mathbb{R}^6)$ into an infinite direct sum of spaces $\mathscr{H}_k$, each left invariant by all of the operators $H_0(\theta)$, $V(\theta)$. For each n and m, $E_{n,m}$ is an eigenvalue of only finitely many of the operators $H_0(\theta) \restriction \mathscr{H}_k$. For some of the $\mathscr{H}_k$, $E_{n,m}$ is nondegenerate. Those $\mathscr{H}_k$ for which $E_{n,m}$ is an eigenvalue of $H_0(\theta) \restriction \mathscr{H}_k$ and those for which it is nondegenerate depend on n and m. Below, we assume that we have restricted to an $\mathscr{H}_k$ on which $E_{n,m}$ is nondegenerate without introducing new notation. We discuss some of the details of the degenerate theory and the reduction by symmetries in the Notes.

Let $H(\theta; \beta) = H_0(\theta) + \beta V(\theta)$. By the theory of regular perturbations described in Section 2, if θ is fixed and $|\beta|$ is sufficiently small, then $H(\theta; \beta)$ has an eigenvalue near $E_{n,m}$ given by a convergent power series in β. See Figure XII.9a,b. Now, let us fix β and vary θ. Since $H(\theta; \beta)$ is an analytic family in θ for β fixed we have an eigenvalue $E^{(\theta)}(\beta)$ *as long as the eigenvalue stays isolated.* $E^{(\theta)}(\beta)$ is analytic in θ for β fixed. Since $H(\theta; \beta)$ and $H(\theta'; \beta)$ are unitarily equivalent if $\theta - \theta'$ is real, $E^{(\theta)}(\beta)$ is constant in θ. We can now prove that $\operatorname{Im} E_{2,2}^{(\theta_0)}(\beta_0) \leq 0$ if β_0 is real and $\operatorname{Im} \theta_0 > 0$. For suppose that $\operatorname{Im} E_{2,2}^{(\theta_0)}(\beta_0) > 0$. Then the eigenvalue stays isolated if we continue θ to 0 keeping $\operatorname{Im} \theta \geq 0$. This would imply $H(0; \beta_0)$ has a complex eigenvalue, which is impossible. We thus conclude that $\operatorname{Im} E_{2,2}^{(\theta_0)}(\beta) \leq 0$. If $\operatorname{Im} E_{2,2}^{(\theta_0)}(\beta) < 0$, and we try to continue θ to zero, the essential spectrum swings into the eigenvalue, invalidating discrete perturbation theory. There is thus no contradiction between the self-adjointness of $H_0 + \beta_0 V$ for β_0 real and the occurrence of complex eigenvalues, $E_{2,2}^{(\theta_0)}(\beta_0)$ in the lower half-plane when β_0 is real and $\operatorname{Im} \theta_0 > 0$.

The second crucial remark is that these complex eigenvalues of $H(\theta; \beta)$ are related to second sheet poles of the resolvent of $H(\beta) = H_0 + \beta V$. Let $\psi \in \mathscr{H}$ be a vector so that $U(\theta)\psi$ has an analytic continuation to all of $\mathbb{C}$. Take ψ to be an entire vector for the infinitesimal generator of the group $U(\theta)$. Consider the function $R_\psi(E) = (\psi, (H_0 + \beta V - E)^{-1}\psi)$ originally defined in the cut plane $\mathbb{C} \backslash \sigma(H_0 + \beta V)$. For θ real,

$$\begin{aligned} R_\psi(E) &= (U(\theta)\psi, U(\theta)(H_0 + \beta V - E)^{-1} U(\theta)^{-1} U(\theta)\psi) \\ &= (U(\theta)\psi, (H(\theta; \beta) - E)^{-1} U(\theta)\psi) \end{aligned}$$

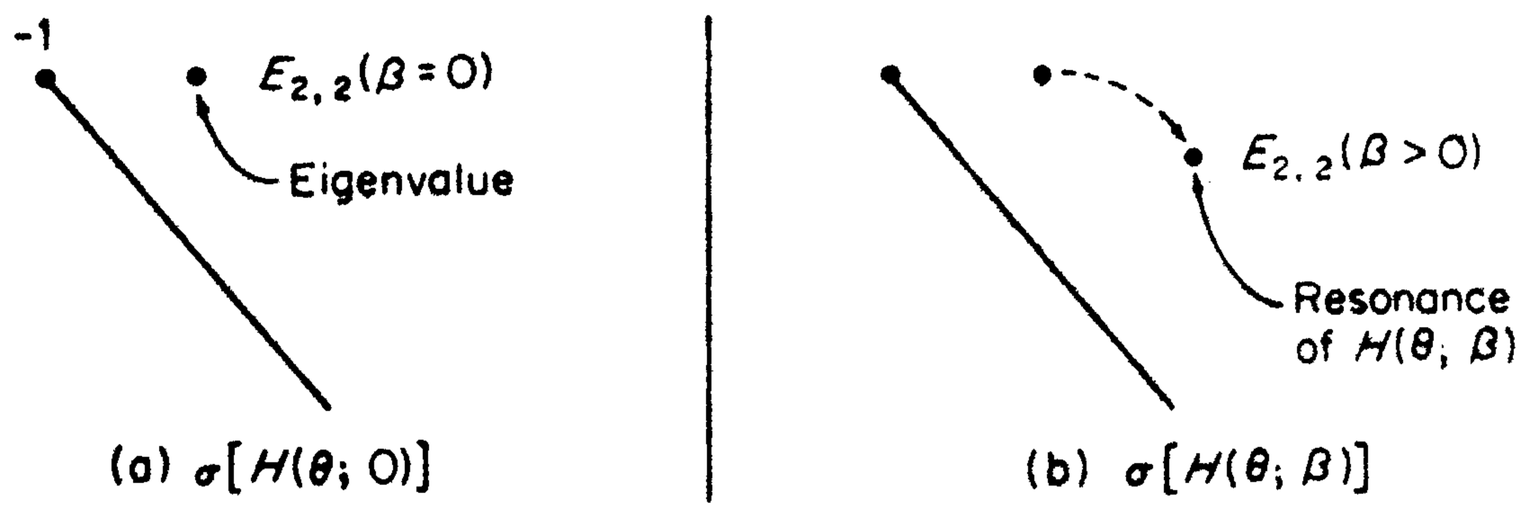
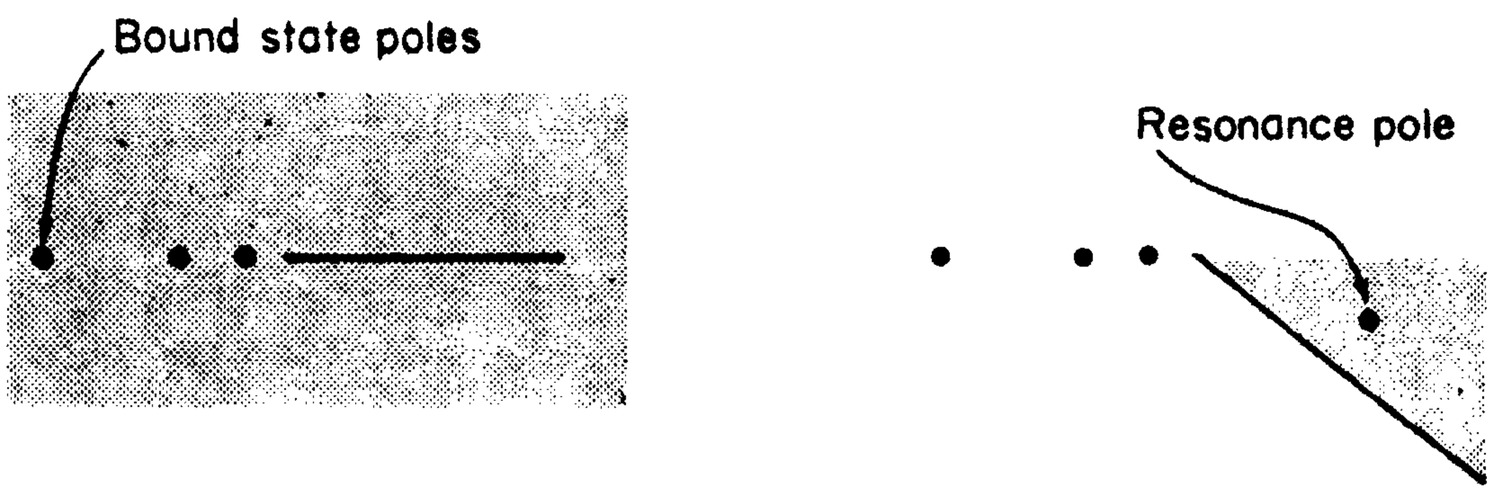


FIGURE XII.9 Trajectory of $E(\beta, \theta)$ for θ fixed; $\operatorname{Im} \theta > 0$.



(a) Original domain

(b) Additional second sheet domain

FIGURE XII.10 Domain of analyticity for $R_\psi(E)$.

Fix E in the upper half-plane. The last formula then holds by analytic continuation if $0 \leq \operatorname{Im} \theta < \frac{1}{2}\pi$. Thus we can continue $R_\psi(E)$ across the real E axis onto parts of the second sheet (Figure XII.10). Since $(H(\theta; \beta) - E)^{-1}$ has poles when E is an eigenvalue of $H(\theta; \beta)$, the analytic continuation of $R_\psi(E)$ will have poles at the complex eigenvalues of $H(\theta; \beta)$. In summary: *The complex eigenvalues of* $H(\theta; \beta)$ *are the positions of second sheet poles of the resolvent.*

The width of these resonance poles is, by definition, the imaginary part of $E^{(\theta)}(\beta)$. $E^{(\theta)}(\beta)$ is in turn given for θ fixed and β small by a convergent perturbation series $\sum_{n=0}^{\infty} a_n \beta^n$. By our basic constancy-in-θ argument, the a_n are independent of θ. Clearly a_0 is real and since $\operatorname{Im} E \leq 0$ for all real β, $\operatorname{Im} a_1 = 0$. a_2 is thus the first a_n for which it is possible that $\operatorname{Im} a_n \neq 0$. If the perturbation series is rapidly convergent, then $|\operatorname{Im} E(\beta)| = \frac{1}{2}\Gamma \approx (\operatorname{Im} a_2)\beta^2$. Thus

$$\Gamma \approx (\beta^2)(2 \operatorname{Im} a_2)$$

a_2 is a Rayleigh–Schrödinger coefficient and can be computed by methods we discussed in Section 1. Explicitly, if $\Omega(\theta; 0)$ is the unperturbed eigenvector of $H(\theta; 0) \equiv H_0(\theta)$ and $\overline{\Omega(\theta; 0)}$ is its complex conjugate as an element of $L^2(\mathbb{R}^6)$, then (Problem 33)

$$a_2 = (2\pi i)^{-1} \oint_{|E - E_0| = \varepsilon} (\overline{\Omega(\theta; 0)}, V[H_0(\theta) - E]^{-1} V\Omega(\theta; 0)) \frac{dE}{E - E_0}$$

where E_0 is the unperturbed eigenvalue. Now consider the function

$$f(\theta, E) = (\overline{\Omega(\theta, 0)}, V(\theta)(H_0(\theta) - E)^{-1} V(\theta)\Omega(\theta; 0)) - |(\overline{\Omega(\theta; 0)}, V(\theta)\Omega(\theta; 0))|^2 (E_0 - E)^{-1}$$

$f(\theta, E)$ is analytic at $E = E_0$ for θ fixed with $\operatorname{Im} \theta > 0$, for we have subtracted the pole term explicitly. Thus by the Cauchy integral theorem,

$$a_2 = f(\theta, E)\Big|_{E = E_0} = \lim_{\varepsilon \downarrow 0} f(\theta, E_0 + i\varepsilon) = \lim_{\varepsilon \downarrow 0} f(\theta = 0, E_0 + i\varepsilon)$$

In the last step we have used the fact that for Im $E > 0$, $f(\theta, E)$ is defined for Im $\theta = 0$ and is independent of θ in the strip $0 \leq \text{Im } \theta < \frac{1}{2}\pi$. Thus

$$\text{Im } a_2 = \lim_{\varepsilon \downarrow 0} \frac{1}{2i} \Big[(\Omega_0 , V\{(H_0 - E_0 - i\varepsilon)^{-1} - (H_0 - E_0 + i\varepsilon)^{-1}\} V\Omega_0)$$

$$- |(\Omega_0 , V\Omega_0)|^2 \{(E - E_0 - i\varepsilon)^{-1} - (E - E_0 + i\varepsilon)^{-1}\} \Big|_{E = E_0} \Big]$$

By the Stone formula (Theorem VII.13), Im a_2 is a function of the spectral projections for H_0 except that the subtraction of the pole subtracts the projection onto the eigenvector Ω_0. We can now prove:

Theorem XII.24 (the Fermi golden rule for Auger states in helium) Let n, m be given with $n > 1$, $m > 1$, and restrict to a symmetry subspace on which $E_{n,m}$ is a nondegenerate eigenvalue. Then, for β real and small, the resolvent of

$$-\Delta_1 - \Delta_2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{\beta}{|r_1 - r_2|}$$

has a second sheet pole near $E_0 \equiv a_0 = -n^{-2} - m^{-2}$. The position of the pole is given by a function $E(\beta)$, which is analytic for β small,

$$E(\beta) = a_0 + a_1 \beta + a_2 \beta^2 + \cdots$$

Let $\{P_\Omega\}$ be the spectral family for $H_0 = -\Delta_1 - \Delta_2 - 2/r_1 - 2/r_2$ and define $\tilde{P}(E) = P_{(-\infty, E)\setminus\{E_0\}}$. Let Ω_0 be the unperturbed eigenvector of H_0. Then:

(a) $g(E) = (\Omega_0 , V\tilde{P}(E)V\Omega_0)$ is analytic at $E = E_0$.

(b) $$\text{Im } a_2 = \pi \frac{dg}{dE}\Big|_{E = E_0}$$

Proof We need only prove (a) and (b) because of our previous discussion. By Stone's formula, to prove (a) and (b) we need only show that

$$(\Omega_0 , V\{(H_0 - E)^{-1} - (E_0 - E)^{-1} P_{\{E_0\}}\} V\Omega_0)$$

has an analytic continuation from the region Im $E > 0$ up to and below the real axis near $E = E_0$. For then $g(E)$ is the integral of an analytic function and its derivative is just (up to a factor of π) the expression we already have for Im a_2. To see that the required function is analytic at $E = E_0$, we need only show that $U(\theta)V\Omega_0$ has an analytic continuation to a strip $|\text{Im } \theta| < \varepsilon$. But

$$U(\theta)V\Omega_0 = [U(\theta)VU(\theta)^{-1}]U(\theta)\Omega_0 = (e^{-\theta}V)[U(\theta)\Omega_0]$$

That $U(\theta)\Omega_0$ has an analytic continuation is an argument using the Schwarz reflection principle (Problem 35). ∎

Thus we have shown that in lowest order perturbation theory,

$$\Gamma = 2 \operatorname{Im} a_2 = 2\pi \frac{d}{dE} (\Omega_0 , V\tilde{P}(E)V\Omega_0) \Big|_{E=E_0}$$

This formula is the Fermi golden rule, written in a slightly different form than is usual in the physics literature.

NOTES

For a wealth of information about the perturbation theory of discrete spectra, see the classic: T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin and New York, 1966 (2nd ed. 1976).

Section XII.1 For additional discussion of the material in this section, see Kato, Chapters I and II, and F. Rellich, *Perturbation Theory of Eigenvalue Problems*, Gordon and Breach, New York, 1969. Theorems XII.1 and XII.2 are discussed, and in particular Theorem XII.2 is proven, in K. Knopp *Theory of Functions*, Part II, Dover, New York, 1947.

Rellich's theorem was first proven in F. Rellich, "Störungstheorie der Spektralzerlegung, I," *Math. Ann.* **113** (1937), 600–619. To appreciate its depth, we note that it is false for analytic perturbations depending on two parameters, as is seen by the following example (a modification of one given by Rellich): Let $T(\beta, \lambda) = \beta\left[\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right] + \lambda\left[\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right]$. $T(\beta, \lambda)$ is analytic in β and λ and self-adjoint for β and λ real, but its eigenvalues $E(\beta, \lambda) = \pm\sqrt{\beta^2 + \lambda^2}$ are not analytic in the two variables β, λ. Rellich's theorem has been extended to various situations involving normal matrices by S. L. Jamison, "Perturbation of normal operators," *Proc. Amer. Math. Soc.* **5** (1954), 103–110, and F. Wolf, "Analytic perturbation of operators in Banach spaces," *Math. Ann.* **124** (1954), 317–333. In particular, Wolf has shown that if $A(\lambda)$ is an analytic family and $A(\lambda_n)$ is normal for a sequence $\lambda_n \to 0$, then the eigenvalues of $A(\lambda)$ are all analytic at $\lambda = 0$. Considerable light has been shed on this theorem by J. Butler, "Perturbation series for eigenvalues of analytic non-symmetric operators," *Arch. Math.* **10** (1959), 21–27; see Problem 21.

For 2×2 matrices, the connection between Jordan anomalous behavior and singularities of the eigenvalues is simple: If $T(\beta) = T_0 + T_1\beta + \cdots + T_n\beta^n + \cdots$ is an analytic 2×2 matrix-valued function with nonanalytic eigenvalues at $\beta = 0$, then for some n, $T_0, \ldots, T_{n-1}$ are multiples of $\mathbb{1}$ and T_n is nondiagonalizable. The general connection is much more complicated; it is implicit in Section II.2.3 of Kato's book; see also Problem 23.

The Rayleigh–Schrödinger series is named for fundamental work of Lord Rayleigh, *The Theory of Sound*, Vol. I, pp. 115–118, MacMillan, London, 1894, and of E. Schrödinger, "Quantisierung als Eigenwertproblem, IV. Störungstheorie mit Anwendung auf den Starkeffekt der Balmerlinien," *Ann. Physik* **80** (1926), 437–490. The projection technique that we use to discuss the Rayleigh–Schrödinger series is due to B. Sz-Nagy in "Perturbations des transformations autoadjointes dans l'espace de Hilbert," *Comment. Math. Helv.* **19** (1946/47), 347–366, and T. Kato in "On the convergence of the perturbation method, I, II" *Progr. Theoret. Phys.* **4** (1949), 514–523; **5** (1950), 95–101; 207–212.

Section XII.2 The original theory of regular perturbations appeared in F. Rellich, "Störungstheorie der Spektralzerlegung I–V," *Math. Ann.* **113** (1937), 600–619, 677–685; **116** (1939), 555–570; **117** (1940), 356–382; **118** (1942), 462–484, with simplifications due to Sz-Nagy and Kato (see the Notes to Section 1). Additional discussion can be found in the books of Rellich and Kato and in the book by K. O. Friedrichs, *Perturbation of Spectra in Hilbert Space*, Amer. Math. Soc., Providence, Rhode Island, 1965.

Our definition of analytic family is slightly different from that used by Kato in his book (p. 366) and by Rellich in the third paper of his series. In case $T(\beta)$ is closed and has a nonempty resolvent set, the definitions agree. The Kato–Rellich definition allows certain cases where $T(\beta)$ may have empty resolvent set; but since such cases rarely arise in practice, we have used a more restrictive but technically simpler definition.

For further discussion of the application of perturbation theory to atomic physics, see M. Mizushima, *Quantum Mechanics of Atomic Spectra and Atomic Structure*, Benjamin, New York, 1970. In particular, references for the hyperfine structure of hydrogen can be found therein.

Theorem XII.10 is proven in B. Simon and R. Höegh-Krohn, "Hypercontractive semigroups and two-dimensional self-coupled Bose fields," *J. Functional Analysis* **9** (1972), 121–180. Another technique for obtaining lower bounds on the radius of convergence of the Rayleigh–Schrödinger series in special cases of physical interest appears in D. Atkinson, "Bound state perturbation theory: A new approach," *Nuclear Phys.* **B20** (1970), 125–158.

Theorem XII.12 was first proven in T. Kato, "On the adiabatic theorem of quantum mechanics," *J. Phys. Soc. Japan* **5** (1950), 435–439. A weaker theorem that suffices for our application of Theorem XII.12 in Theorem XII.13 can be found in the paper of Sz-Nagy mentioned in the Notes to Section 1. Sz-Nagy gives an explicit formula for an invertible operator $W(\beta)$ defined for $|\beta|$ sufficiently small with $W(\beta)P(0)W(\beta)^{-1} = P(\beta)$. Namely (see Problem 19)

$$W(\beta) = [1 - (P(\beta) - P(0))^2]^{-1/2}[P(\beta)P(0) + (1 - P(\beta))(1 - P(0))]$$

The lemma to Theorem XII.12 can also be proven using fixed point theorems.

Section XII.3 The heuristic argument for the divergence of the perturbation series for the anharmonic oscillator is discussed in K. Gottfried, *Quantum Mechanics*, vol. I, pp. 361–362, Benjamin, New York, 1966. The model for all such heuristic arguments was given by F. Dyson, "Divergence of perturbation theory in quantum electrodynamics," *Phys. Rev.* **85** (1952), 631–632.

The detailed estimate necessary for proving divergence of the series ($|a_n| \geq AB^n\Gamma(n/2)$) is proven in C. Bender and T. T. Wu, "Anharmonic oscillator," *Phys. Rev.* **184** (1969), 1231–1260. Their proof is modeled on an analogous proof for the $(\varphi^4)_2$-field theory which is found in A. M. Jaffe, "Divergence of perturbation theory for bosons," *Comm. Math. Phys.* **1** (1965), 127–149.

The nature of the singularity of the anharmonic oscillator eigenvalues at $\beta = 0$ has been studied in detail. $E(\beta)$ has an analytic continuation to a three-sheeted surface on which $\beta = 0$ is *not* an isolated singularity. This was first suggested by approximate calculations of Bender and Wu (see above) and proven in B. Simon, "Coupling constant analyticity for the anharmonic oscillator," *Ann. Phys.* **58** (1970), 76–136.

A particularly clear discussion of the Gell'Mann–Low series and its *formal* derivation in quantum field theory may be found in J. Bjorken and S. Drell, *Relativistic Quantum Fields*, McGraw-Hill, New York, 1965. For a discussion of the general theory of asymptotic series, see W. Wasow, *Asymptotic Series for Ordinary Differential Equations*, Wiley (Interscience), New York, 1965. The table in Example 1 comes from the *Ann. Phys.* article by Simon.

That perturbation series are asymptotic was first proven by E. Titchmarsh, "Some theorems

on perturbation theory, I, II," *Proc. Roy. Soc.* **A200** (1949), 34–46; **A201** (1950), 473–479. Extensions of Titchmarsh's results are due to T. Kato, "On the convergence of the perturbation method," *J. Fac. Sci. Univ. Tokyo Sect. I*, **6** (1951), 145–226, and "Perturbation theory of semi-bounded operators," *Math. Ann.* **125** (1953), 435–447, and by V. Kramer "Asymptotic inverse series," *Proc. Amer. Math. Soc.* 7 (1956), 429–437, and "Asymptotic perturbation series," *Trans. Amer. Math. Soc.* **85** (1957), 88–105.

Some generalizations of the Titchmarsh results to nonsymmetric operators may be found in D. Huet, "Phénomènes de perturbation singulière," *C. R. Acad. Sci. Paris* **244** (1957), 1438–1440; **246** (1958), 2096–2098; **247** (1958), 2273–2276; **248** (1959), 58–60; and "Phénomènes de perturbation singulière dans les problèmes aux limites," *Ann. Inst. Fourier* **10** (1960), 1–96. An alternative method of proving perturbation series asymptotic which is applicable to positive self-adjoint perturbations of positive self-adjoint operators is discussed in Appendix II of Simon's *Ann. Phys.* article and in W. M. Greenlee, "Singular perturbation of eigenvalues," *Arch. Rational Mech. Anal.* **34** (1969), 143–164.

Asymptotic perturbation theory is discussed in Chapter VIII of Kato's book. Kato emphasizes that only stability of the eigenvalue and strong resolvent convergence is required; see our discussion of Theorem XII.16.5.

Theorems XII.15 and XII.16 are discussed and proven in B. Simon "Determination of eigenvalues by divergent perturbation series," *Advances in Math.* 7 (1971), 240–253.

The asymptotic nature of the perturbation series for spatially cutoff $(\varphi^{2n})_2$ field theories in sectors $\{\beta \,|\, |\arg \beta| \leq \theta\}$ for $\theta < \pi/2$ was first proven in the paper of B. Simon and R. Hoegh-Krohn, quoted in the Notes to Section 2. The extension to $\theta < \pi$ for $(\varphi^4)_2$ (using Theorem XII.15) first appeared in B. Simon, "Borel summability of the ground state energy in spatially cutoff $(\varphi^4)_2$," *Phys. Rev. Lett.* **25** (1970), 1583–1586. The extension to $\theta < \pi$ for general $(\varphi^{2n})_2$ theories is due to L. Rosen and B. Simon "The $(\varphi^{2n})_2$ Hamiltonian for complex coupling constant," *Trans. Amer. Math. Soc.* **165** (1972), 365–379. Various objects in the infinite volume $P(\varphi)_2$ field theory have been shown to have asymptotic series; see J. Dimock, "Asymptotic perturbation expansions in the $P(\varphi)_2$ quantum field theory," *Comm. Math. Phys.* **35** (1974), 347–356, for the earliest result of this sort.

There is a formal relation between vacuum energies and sums of connected Feynman diagrams with no external legs (see the book of Bjorken and Drell mentioned above). If one modifies the Feynman rules by placing a Fourier transform of g, the spatial cut-off, "at the vertex" instead of a δ function, one obtains the Rayleigh–Schrödinger series for the vacuum energy after explicitly doing the integrals over time.

The double well potential has evoked considerable interest. Previous work includes that of M. Kac and C. Thompson, "Phase transitions and eigenvalue degeneracy of a one dimensional anharmonic oscillator," *Stud. Appl. Math.* **48** (1969), 257–264, and D. Isacson, "The critical behavior of $(\phi^4)_1$," *Commun. Math. Phys.* (to appear). In particular Kac and Thompson prove that $E_i' - E_i$ goes to zero as $\exp(-b\beta^{-2})$. There has also been theoretical work on the question of Borel summability for the double well problem. E. Berezin, G. Parisi, and J. Zinn-Justin, in "Perturbation Theory at large orders for potentials with degenerate minima," *Phys. Rev.* **D16** (1977), 408 study the large n behavior of the Rayleigh–Schrödinger coefficients both numerically and using some not-yet-rigorous theory. Their results suggest that the series will not be Borel summable and this has been proven by A. Sokal, Princeton preprint, 1977.

There is an exactly soluble example similar to the double well potential discussed on pages 66–77 of E. Merzbacher, *Quantum Mechanics*, Wiley, New York, 1961, and pages 12–14 of U. P. Maslov, *Théorie des Perturbations et méthods Asymptotiques*, Dunod and Gauthier-Villars, Paris, 1972.

The special interest in the double well comes from the rather different behavior of the

correspondng two-dimensional field theory. In the double well problem, even though $E_0' - E_0$ is small, it is nonzero and the ground state is symmetric about $x = -\frac{1}{2}\beta^{-1}$. In the corresponding field theory, if one chooses the limit theory which is symmetric, then the vacuum is degenerate and the (decomposed) theories with unique vacuum do not have the symmetry. This has been proven by J. Glimm, A. Jaffe, and T. Spencer, "Phase transitions for ϕ_2^4 quantum fields", *Commun. Math. Phys.* **45** (1975), 203–216. This distinction between one and two dimensions is analogous to the fact that the Ising model has a phase transition in two but not in one dimension; we return to these matters in a later volume.

Section XII.4 Carleman's theorem (Theorem XII.17) is proven in *Les Fonctions Quasi Analytiques*, Gauthier-Villars, Paris, 1926. The method of proof for the general case is very different from the special case given as Theorem XII.18. Our proof of Theorem XII.18 follows that given by G. H. Hardy, *Divergent Series*, Oxford Univ. Press, London and New York, 1949.

The idea of applying the notion of the strong asymptotic condition to divergent perturbation series, and in particular its application to the anharmonic oscillator, is due to S. Graffi, V. Grecchi, and B. Simon, "Borel summability: Application to the anharmonic oscillator," *Phys. Lett.* **32B** (1970), 631–634. Theorem XII.20 was first stated and proven in Simon's *Advances in Math.* paper quoted in the Notes to Section 3, and Example 2 was first discussed in Simon's *Phys. Rev. Lett.* article also mentioned in the above Notes. Basic references for two-dimensional Bose field theories are discussed in the Notes to Section X.7. Example 3 (x^{2n} oscillator) was first discussed in the above-mentioned paper by Graffi *et al.* It has been shown that certain asymptotic series for infinite volume $P(\varphi)_2$ theories are Borel summable. See J.-P. Eckmann, J. Magnen, and R. Sénéor, "Decay properties and Borel summability for the Schwinger functions in $P(\varphi)_2$ theories," *Comm. Math. Phys.* **39** (1975), 251–271. The perturbation series for the Zeeman effect (an atom in a constant magnetic field) has been proven to be Borel summable by J. Avron, I. Herbst, and B. Simon, "Schrödinger Operators with Magnetic Fields," 1977 preprint.

Watson's Theorem was first proven in G. Watson, "A theory of asymptotic series," *Philos. Trans. Roy. Soc. London Ser. A* **211** (1912), 279–313. Borel first proposed his method and showed that it worked in many examples in "Mémoire sur les séries divergentes," *Ann. Sci. École Norm. Sup.* **16** (1899), 9–136.

The Borel method is an example of a regular summability method. A summability method is a procedure for defining a sum α for certain formal series $\sum a_n$. The method is called regular if, whenever $\sum a_n$ is absolutely convergent to α_0, the procedure is applicable and yields α_0 as sum. The regularity of the Borel method, which follows from Watson's theorem, was first proven by G. Hardy, "On differentiation and integration of divergent series," *Trans. Cambridge Phil. Soc.* **19** (1904), 297–321.

One disadvantage of the Borel method, as it stands, is that it involves an analytic continuation that can be difficult to do computationally. This difficulty can be overcome by finding a conformal map that takes the region of analyticity given by Watson's theorem into a region including a unit circle in such a way that the image of the positive reals lies in this circle. One can then do the "continuation" by merely summing a power series in the image region. For additional details, see N.-E. Nörlund, *Leçons sur les séries d'interpolation*, Gauthier-Villars, Paris, 1926; G. Doetsch, *Handbuch der Laplace-Transformation*, Birkhäuser, Basel, 1955, Vol. 2, Chap. 11; B. Hirsbrunner and J. Loeffel, "Sur les séries asymptotiques sommables selon Borel," *Helv. Phys. Acta* **48** (1975), 546. The last reference contains an application to x^4 oscillators.

Another summability method, the method of Padé approximants, is known to correctly "sum" the perturbation series for x^4 and x^6 perturbations of $p^2 + x^2$. This method is discussed

in G. A. Baker, "The theory and application of the Padé approximant method," *Advances Theoret. Phys.* **1** (1966), 1–58. The applicability of the method (which is not known to be regular) to x^4 and x^6 oscillators is proven in J. J. Loeffel, A. Martin, B. Simon, and A. S. Wightman, "Padé approximants and the anharmonic oscillator," *Phys. Lett.* **30B** (1969), 656–658. The advantage of the Padé method is its computational simplicity; one has explicit formulas for the approximants and explicit control on the errors. Its disadvantages are its limited applicability (numerical evidence suggests that it does not work for an x^8 oscillator) and the difficulty of proving convergence (it has not been proven that the method works for two-dimensional x^4 oscillators). The reader should compare the partial sums of the Rayleigh–Schrödinger series for the ground state of $p^2 + x^2 + 0.2x^4$ (exact value: $E_0 = 1.118292$) given in Section 3 with the $[N, N]$ Padé approximants:

$$\begin{aligned} E[1,1] &= 1.111111 & E[5,5] &= 1.118288 \\ E[2,2] &= 1.117541 & E[6,6] &= 1.118292 \\ E[3,3] &= 1.118183 & E[7,7] &= 1.118292 \\ E[4,4] &= 1.118272 \end{aligned}$$

The $[N, N]$ Padé approximant is computed using only the Rayleigh–Schrödinger coefficients $a_0, \ldots, a_{2N}$.

There is a family of perturbations of the discrete spectrum that leaves the spectrum discrete but which is more singular than anything we have discussed thus far. Typical of this class is $H_0 = -d^2/dx^2 + x^2$ on $L^2(\mathbb{R}, dx)$, where $V = x^{-\alpha}$. For $\alpha > 1$, this family is discontinuous at $\lambda = 0$ if $H_0 + \lambda V$ is defined as a form sum. Explicitly, $H_0 + \lambda V$ converges as $\lambda \downarrow 0$ in strong resolvent sense to an operator $\tilde{H}_0$ different from H_0. This phenomenon was discovered by J. Klauder, "Field structure through models studies," *Acta Phys. Austriaca. Supp.* **11** (1973), 341–387, and is further discussed by B. Simon, "Quadratic forms and Klauder's phenomenon: A remark on very singular perturbations," *J. Functional Analysis* **14** (1973), 295–298, and B. DeFacio and C. L. Hammer, "Remarks on the Klauder phenomenon," *J. Mathematical Phys.* **15** (1974), 1071–1077. If $H(\lambda)$ is set equal to $\tilde{H}_0$ when $\lambda = 0$, then the resulting family is analytic at $\lambda = 0$ so long as $1 \leq \alpha < 2$. For $2 \leq \alpha < 3$, the eigenvalues are given by asymptotic series to first order so long as $\lambda > 0$. But for $\alpha \geq 3$, the eigenvalues approach those for $\tilde{H}_0$ more slowly than linearly in λ. Explicitly, for $\alpha > 3$,

$$E(\lambda) - E(0) = c\lambda^{1/(\alpha-2)} + o(\lambda^{1/(\alpha-2)})$$

for $c \neq 0$, and for $\alpha = 3$,

$$E(\lambda) - E(0) = c\lambda \ln \lambda + O(\lambda)$$

These phenomena are further discussed in J. Klauder and L. Detwiler, "Supersingular quantum perturbations," *Phys. Rev.* **D11** (1975), 1436–1441 and in W. Greenlee, "Singular perturbation theory for semi-bounded operators," *Bull. Amer. Math. Soc.* **82** (1976), 341–344, and E. Harrell, II, "Singular Perturbation Potentials," *Ann. Phys.* **105** (1977), 379–406.

Section XII.5 That Schrödinger's theory of the Stark effect was not entirely satisfactory due to the occurrence of continuous spectrum in $(-\infty, \infty)$ was first pointed out by J. R. Oppenheimer in "Three notes on the quantum theory of aperiodic effects," *Phys. Rev.* **31** (1928), 66–81. One interpretation of this perturbation series, which we shall discuss below, is expounded in E. C. Titchmarsh "Some theorems on perturbation theory, III, IV, V," *Proc. Roy. Soc.* **A207** (1951), 321–328; **A210** (1951), 30–47; *J. Analyse Math.* **4** (1954/56), 187–208. In the last paper, "spectral concentration" was defined.

Progress toward the isolation of the notions and relations of spectral concentration and pseudo-eigenvectors was made due to work of K. Friedrichs, "Über die Spektralzerlegung eines Integraloperators," *Math. Ann.* **115** (1938), 249–272; and "On the perturbation of continuous spectra," *Comm. Pure Appl. Math.* **1** (1948), 361–406; T. Kato's *J. Fac. Sci. Univ. Tokyo* paper quoted in the notes to Section 3 and K. Friedrichs and P. Rejto, "On a perturbation through which a discrete spectrum can become continuous," *Comm. Pure Appl. Math.* **15** (1962), 219–235. The pth order analogue of Theorem XII.22 is due to R. C. Riddell, "Spectral concentration for self-adjoint operators," *Pacific J. Math.* **23** (1967), 377–401. Independently, one half of the extended theorem (that a pth order pseudo-eigenvector implies pth order spectral concentration) and all of Theorem XII.22 were proven by C. C. Conley and P. A. Rejto, "Spectral concentration II: General theory," in *Perturbation Theory and its Application in Quantum Mechanics* (C. H. Wilcox, ed.) Wiley, New York, 1966. Our proof of Theorem XII.23 follows that of Conley and Rejto, where there is also a detailed discussion of the Stark effect in order $p > 1$. For additional discussion of the theory of spectral concentration and some additional applications, see K. Veselić, "On spectral concentration for some classes of self-adjoint operators," *Glasnik Math. Ser. III* **4** (1969), 213–228 and "The nonrelativistic limit of the Dirac equation and spectral concentration," *Glasnik Math. Ser. III* **4** (1969), 231–240. In the last paper Veselić considers the Dirac Hamiltonian $H = H_0 + V(x) - mc^2$ where $V(x) \to \infty$ as $|x| \to \infty$. H has continuous spectrum in $(-\infty, \infty)$ for any c since the negative energy states see an effective potential going to $-\infty$ as $|x| \to \infty$. As $c \to \infty$, H has spectral concentration about the eigenvalues of $-\Delta + V$.

For a discussion of the spectral properties of the Stark effect Hamiltonian, see Section XIII.4, Example 8, and the Notes to that section.

For a class of models closely related to the Stark effect but having spherical symmetry so that ordinary differential equation methods are applicable (examples: $-d^2/dx^2 + |x| - \beta x^2$ and $-\Delta - 1/r - \beta|r|$), Titchmarsh found the following phenomena: H has continuous spectrum concentrated about pseudo-eigenvalues (for $\beta > 0$ in the two examples), but the pseudo-eigenvalues have a stronger meaning—the Green's function (kernel of the resolvent) has an analytic continuation below the real axis with a pole at $E(\beta)$ on the second sheet. Re $E(\beta)$ has the Rayleigh–Schrödinger series as asymptotic series, and Im $E(\beta)$ goes to zero faster than any β^n. This is to be compared with the phenomena discussed in Section 6. There is a second sheet pole in both cases, but in one case (Stark effect) the width is $o(\beta^n)$ for all n and in the other (Auger effect) it is $O(\beta^2)$. This is mirrored in the degree of spectral concentration: In one case (Stark effect) there is concentration to all orders and in the other case to second order and not to higher order (we discuss spectral concentration in this Auger case in the Notes to Section 6).

We note that in some physics literature, the imaginary part of this second sheet pole is called the "natural" width. There is also a contribution to the observed width due to the interaction with the radiation field (radiative width) and a contribution due to the thermal motion of the sources (thermal width or Doppler width).

Spectral concentration for the Stark effect in helium has been studied by P. Rejto in "Second order concentration near the binding energy of the helium Schrödinger operator," *Israel J. Math.* **6** (1968), 311–337, and "Spectral concentration for the helium Schrödinger operator," *Helv. Phys. Acta* **43** (1970), 652–667. Given Theorems X.38 and XIII.39, it is easy to verify the hypotheses of Theorem XII.22 in this case.

In discussing spectral concentration in electric fields, it is useful to know that the eigenfunctions of H_0 fall off faster than inverse polynomials in the sense that $\psi \in D(r^n)$ for all n. Results of this sort are proven in Section XIII.11.

There is a case where eigenvalues get "absorbed" by the continuous spectrum which is much less singular than the situations described in this section. This is the situation of an analytic

family of type (A) where a discrete eigenvalue approaches the continuous spectrum as β approaches some critical coupling constant. Some information in this case may be found in B. Simon, "On the absorption of eigenvalues by continuous spectrum in regular perturbation problems," *J. Functional Analysis* (to appear).

Section XII.6 The association of resonances with second sheet poles in the scattering amplitude is an idea that was introduced in the early days of quantum mechanics by V. Weisskopf and E. P. Wigner "Berechnung der natürlichen Linienbreite auf Grund der Diracschen Lichttheorie," *Z. Phys.* **63** (1930), 54–73. The idea of looking instead at poles in the resolvent is a later refinement explicitly discussed by J. Schwinger, "Field theory of unstable particles," *Ann. Phys.* **9** (1960), 169–193; C. Lovelace, "Three particle systems and unstable particles," in *Strong Interactions and High Energy Physics: 1963 Scottish Universities' Summer School* (R. C. Moorhouse, ed.), Oliver and Boyd, 1964; and A. Grossman, "Nested Hilbert space in quantum mechanics, I," *J. Mathematical Phys.* **5** (1964), 1025–1037. There is, of course, a connection between this idea and the work of Titchmarsh described at the end of the Notes to Section 5.

Many of the earliest attempts at understanding resonances from a rigorous point of view involved ad hoc non-self-adjoint models, often with $H^* - H$ compact. Typical is M. Livsic, "The method of non-self-adjoint operators in dispersion theory," *Uspehi Mat. Nauk.* **12** (1957) [English translation: *Amer. Math. Soc. Transl. Ser. 2* **16** (1960), 427–433]. A summary of various attempts along these lines may be found in C. L. Dolph, "Recent developments in some non-self-adjoint problems of Mathematical Physics," *Bull. Amer. Math. Soc.* **67** (1961), 1–69.

Attempts at finding second sheet poles and related phenomena such as spectral concentration in the resolvents of self-adjoint operators obtained from perturbing operators with eigenvalues in the continuum were made by Friedrichs in his *Comm. Pure Appl. Math.* paper (see Notes to Section 5) and by J. S. Howland in a series of papers: "Perturbation of embedded eigenvalues by operators of finite rank," *J. Math. Anal. Appl.* **23** (1968), 575–584; "Embedded eigenvalues and virtual poles," *Pacific J. Math.* **29** (1969), 565–582; "Spectral concentration and virtual poles," *Amer. J. Math.* **91** (1969), 1106–1126; "On the Weinstein–Aronszajn formula," *Arch. Rational Mech. Anal.* **39** (1970), 323–339. All these papers use models where the perturbation is compact (and even finite rank in most cases). The perturbations of Section 6 are not even relatively compact. Recently (and approximately simultaneously to the work of Simon mentioned below), Howland has extended Friedrichs' method to treat models similar to the autoionizing model. This work is discussed in J. S. Howland "Perturbation of embedded eigenvalues" *Bull. Amer. Math. Soc.* **78** (1972), 380–383, and "Puiseux Series for Resonances at an Embedded Eigenvalue," *Pacific J. Math.* **55** (1974), 157–176. In the latter article, Howland shows that Rellich's theorem does not extend to resonance theory, i.e., one can have H_0 and V self-adjoint and an embedded degenerate eigenvalue E_0 of H_0 where $H_0 + \beta V$ has resonance at values $E_n(\beta)$ where the $E_n(\beta)$ are not analytic at $\beta = 0$ but have a Puiseux series with fractional terms. Howland has also explained how the notion of resonance associated with an embedded eigenvalue of H_0 is intrinsic to the pair $\{H_0, V\}$.

The basic technique sketched in this section is developed in Section XIII.10. Detailed references can be found in the notes to that section. Our discussion here is largely taken from B. Simon, "Resonances in N-body quantum systems with dilatation analytic potentials and the foundations of time-dependent perturbation theory," *Ann. Math.* **97** (1973), 247–274.

The reduction due to symmetry is described in Simon's paper. Basically, the idea is the following. H_0 and V both commute with rotations and the reflection P through the origin. Thus, they also commute with the generators J_x, J_y, J_z of rotations about the x, y, and z axes (angular momentum operators). The operators P, J_z, and $J^2 \equiv J_x^2 + J_y^2 + J_z^2$ commute with one another

and all have discrete spectrum. Thus, $\mathscr{H}$ breaks up into a direct sum $\bigoplus \mathscr{H}_{p,j,m}$ with $p = \pm 1$, $j = 0, 1, 2, \ldots$, and $m = -j, -j+1, \ldots, j-1, j$, so that if $\psi \in \mathscr{H}_{p,j,m}$, then

$$P\psi = p\psi, \qquad J^2\psi = j(j+1)\psi, \qquad J_z\psi = m\psi$$

H_0 and V leave each $\mathscr{H}_{p,j,m}$ invariant.

For the case of the helium atom, we saw that $\sigma_{ess}(H_0) = [-1, \infty)$. However, it turns out that $\sigma_{ess}(H_0 \restriction \mathscr{H}_{p,j,m}) = [-\frac{1}{4}, \infty)$ if $p = (-1)^{j+1}$ so that certain eigenvalues of H_0 lying in $[-1, -\frac{1}{4})$ that appear embedded are not embedded once the symmetry reduction is made. Of course, these eigenvalues do not disappear when the perturbation is turned on. It is expected that all other eigenvalues do disappear—the method of this section reduces the proof of this to explicitly evaluating Im a_2 to see if it is nonzero.

Spectral concentration has been studied in situations where a "virtual pole" (second sheet pole) of the resolvent of $H_0 + \beta V$ occurs at $E(\beta)$ with $E(0)$ a real eigenvalue of H_0 and $E(\beta)$ analytic. In a family of models, Howland studied the question in his *Pacific J. Math.* paper quoted above. In the Auger problem, Simon has studied the question (in the above reference). The result, related to the fact that Im $E = O(\beta^2)$, is that there is spectral concentration to first order: Explicitly, $P^{(H_0+\beta V)}(E_0 + \beta E_1 - f(\beta), E_0 + \beta E_1 + f(\beta)) \to P_{(E_0)}$ strongly if and only if $f(\beta) \to 0$ and $f(\beta)/\beta^2 \to \infty$ (so, in some sense, there is concentration to order p for fractional $p < 2$).

Finally, let us summarize the "usual" physical (and *nonrigorous*) argument leading to the Fermi golden rule: This will enable us to understand how the formula

$$\Gamma = 2\pi \frac{d}{dE}(\Omega_0, V\tilde{P}(E)V\Omega_0)$$

is the Fermi formula, which is usually written in a more formal way. For further discussion of this derivation, see L. Landau and E. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory*, pp. 140–153, Addison-Wesley, Reading, Massachusetts, 1958. One first needs to think of the bump as due to a "virtual process." That is, one pretends there actually are "bound states" near the energies E_n of H_0 which lie in the continuum. These states have characteristic lifetimes τ_n. Thus the scattering process $e + \mathrm{He}^+ \to e + \mathrm{He}^+$ is viewed as $e + \mathrm{He}^+ \to \mathrm{He} \to e + \mathrm{He}^+$. A state of helium is formed and decays in time τ_n. This state has a definite energy E_n, but due to the uncertainty principle the initial energy E of $e + \mathrm{He}^+$ need not be exactly E_n for the state to form. Only $\Delta E = E - E_n$ must be of order $1/\tau_n$ (we have taken $\hbar = 1$). Thus the bump due to formation of the excited state of helium has a characteristic width, $\Gamma_n \equiv \tau_n^{-1}$. Once the state of energy E_n is formed, it decays with a $|P_\ell(\cos\theta)|^2$ distribution if ℓ is the angular momentum of the resonance and if the final state of the He^+ ion is its ground state. As a result, the scattering cross section is enhanced by the occurrence of the resonance.

Now let φ_n be the bound state of H_0 at energy E_n. Suppose H_0 has "continuum eigenfunctions" $\varphi(E)$ with $H_0\varphi(E) = E\varphi(E)$ and $\int \varphi(E)(\varphi(E), \eta)\, dE = \eta$ for any $\eta \in \mathscr{H}$. Let us try to solve the Schrödinger equation $i\dot{\psi} = (H_0 + V)\psi$ with $\psi(0) = \varphi_n$. Write

$$\psi(t) = \int a(E; t)\varphi(E)e^{-iEt}\, dE + \sum a_k(t)e^{-iE_kt}\varphi_k$$

The probability of $\psi(t)$ not being in the state φ_n at time t (i.e., the probability of decay) is given by

$$P(t) = \int |a(E; t)|^2\, dE + \sum_{k \neq n} |a_k(t)|^2$$

Formally, $a(E; t)$ and $a_k(t)$ obey the differential equations

$$i\dot{a}(E; t) = \int a(E'; t)(\varphi(E), V\varphi(E'))e^{-i(E'-E)t}\,dE' + \sum_k (\varphi(E), V\varphi_k)e^{-i(E_m-E)t}a_k(t)$$

$$i\dot{a}_m(t) = \int a(E', t)(\varphi_m, V\varphi(E'))e^{-i(E'-E_m)t}\,dE' + \sum_k (\varphi(E), V\varphi_k)e^{-i(E_m-E)t}a_k(t)$$

Formally, solve these equations in "powers of V." To lowest order ($V = 0$), we have $a(E; t) = 0$, $a_m(t) = 0$ if $m \neq n$, $a_n(t) = 1$. Thus to first order

$$i\dot{a}^{(1)}(E; t) = e^{-i(E_m-E)}(\varphi(E), V\varphi_m)$$

and similarly for a_k. Thus

$$a^{(1)}(E; t) = (\varphi(E), V\varphi_n)\left(\frac{e^{-i(E_n-E)t} - 1}{(E_n - E)}\right)$$

or

$$P^{(1)}(t) = t\int |(\varphi(E), V\varphi_n)|^2\left(\frac{4\sin^2[(t/2)(E_n - E)]}{t(E_n - E)^2}\right)dE$$

$$+ \text{a discrete sum.}$$

As $t \to \infty$,

$$\frac{4\sin^2((t/2)x)}{2\pi t x^2} \to \delta(x)$$

in the sense of distributions, so we can write

$$\lim_{t\to\infty}\frac{P^{(1)}(t)}{t} = 2\pi|(\varphi(E), V\varphi_n)|^2\Big|_{E=E_n}$$

But to lowest order, $\Gamma = \lim_{t\to\infty} t^{-1}P^{(1)}(t)$. Thus

$$\Gamma = 2\pi|(\varphi(E), V\varphi_n)|^2\Big|_{E=E_n}.$$

This is the Fermi golden rule in its more usual form. Sometimes, even more formally, one writes $P_{n\to E}(t) = |a(E; t)|^2$, $\Gamma_{n\to E} = \lim_{t\to\infty} t^{-1}|a(E; t)|^2$, $\Gamma = \int \Gamma_{n\to E}\,dE$ and

$$\Gamma_{n\to E} = 2\pi|(\varphi(E), V\varphi_n)|^2\ \delta(E - E_n)$$

To see that this is just a formal version of our result in Section 6, we note that formally speaking,

$$\tilde{P}(-\infty, E') = \int_{-\infty}^{E'} dE(\varphi(E), \cdot)\varphi(E)$$

Thus

$$\frac{d}{dE'}(V\varphi_n, \tilde{P}(-\infty, E')V\varphi_n)\Big|_{E'=E_n} = (V\varphi_n, \varphi(E'))(\varphi(E'), V\varphi_n)\Big|_{E'=E_n}$$

$$= |(V\varphi_n, \varphi(E'))|^2\Big|_{E'=E_n}$$

PROBLEMS

†1. (a) Suppose that $f_0, f_2, f_3, \ldots, f_n$, and f_1^{-1} are all analytic in $\{\beta \mid |\beta - \beta_0| \leq R_0\}$. Let the α_k be determined by recursive substitution of $\lambda = \lambda_0 + \sum_{k=1}^{\infty} \alpha_k(\beta - \beta_0)^k$ in (1). Prove that $|\alpha_k| \leq AR^k$ for suitable A and R.

(b) Prove that any analytic function $\lambda(\beta)$ with $\lambda(\beta_0) = \lambda_0$ solving (1) near $\beta = \beta_0$ is equal to $\lambda_0 + \sum_{k=1}^{\infty} \alpha_k(\beta - \beta_0)^k$ near $\beta = \beta_0$.

†2. Let T be a matrix written in Jordan normal form with λ_0 an eigenvalue of T. Suppose that ε is so small that λ_0 is the only eigenvalue of T in $\{\lambda \mid |\lambda - \lambda_0| \leq \varepsilon\}$. Prove that

$$P = -(2\pi i)^{-1} \oint_{|\lambda - \lambda_0| = \varepsilon} (T - \lambda)^{-1}\, d\lambda$$

is the projection onto $\{v \mid (T - \lambda_0)^n v = 0 \text{ for some } n\}$ and $Pw = 0$ if $(T - \lambda_1)^n w = 0$ for $\lambda_1 \neq \lambda_0$. (Hint: Prove that $(a^{-1})_{ij} = b_{ij}$ with

$$a_{ij} = (\mu - \lambda)\,\delta_{ij} + \delta_{i+1,j}$$

$$b_{ij} = (\mu - \lambda)^{-1} - (\mu - \lambda)^{-2}\,\delta_{i+1,j} + (\mu - \lambda)^{-3}\,\delta_{i+2,j} - \cdots).$$

3. Let T be a finite matrix. Let 0 be an eigenvalue of T.

(a) Prove that $(T - \lambda)^{-1}$ is analytic in $\{\lambda \mid 0 < |\lambda| < R\}$ for some R and that there are operators A_n so that $(T - \lambda)^{-1} = \sum_{n=-\infty}^{\infty} A_n \lambda^n$ with the sum converging if $0 < |\lambda| < R$.

(b) Prove that $A_n = (2\pi i)^{-1} \oint_{|\lambda| = \varepsilon} \lambda^{-n-1}(T - \lambda)^{-1}\, d\lambda$ for $0 < \varepsilon < R$.

*(c) Use (b) to prove that $A_n A_m = (\eta_n + \eta_m - 1)A_{n+m+1}$ where

$$\eta_n = \begin{cases} 1, & n \geq 0 \\ 0, & n < 0 \end{cases}$$

(Hint: See the proof of Theorem XII.5.)

(d) Let $P = -A_{-1}$; $N = -A_{-2}$; $S = A_0$. Prove that $A_n = S^{n+1}$ for $n \geq 0$, $A_{-n} = -N^{n-1}$ for $n \geq 2$ and that $P^2 = P$; $PN = NP = N$; $PS = SP = 0$.

(e) Prove that $\sum_{n=0}^{\infty} \zeta^n N^n$ converges for all $|\zeta| < \infty$. (Hint: Use (a).)

*(f) Prove that $N^k = 0$ for some k.

(g) Prove that $TP = PT = N$.

4. Let T be an $n \times n$ matrix. Let $\lambda_1, \ldots, \lambda_\ell$ be its eigenvalues. Let

$$P_i = -(2\pi i)^{-1} \oint_{|\lambda - \lambda_i| = \varepsilon_i} (T - \lambda)^{-1}\, d\lambda$$

and

$$N_i = -(2\pi i)^{-1} \oint_{|\lambda - \lambda_i| = \varepsilon_i} (\lambda - \lambda_i)(T - \lambda)^{-1}\, d\lambda.$$

(a) By mimicking Problem 3, prove that $P_i^2 = P_i$; $N_i P_i = P_i N_i = N_i$; $TP_i = P_i T = \lambda_i P_i + N_i$.

*(b) Prove that $P_i P_j = 0$ if $i \neq j$ and $\sum_{i=1}^{\ell} P_i = 1$.

(c) (abstract Jordan normal form). Prove that

$$T = \sum_{i=1}^{\ell} (\lambda_i P_i + N_i)$$

(d) Let N be nilpotent, i.e., $N^k = 0$ for some k. Show that there is a basis for the underlying vector space for which N has the matrix form

$$N = \begin{bmatrix} 0 & x & 0 & \cdots & 0 \\ 0 & 0 & x & \cdots & 0 \\ & & & \ddots & \ddots \\ 0 & 0 & 0 & \cdots & x \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

where each x is equal to 1 or 0.

(e) Show that in a suitable basis T has the Jordan normal matrix form discussed in Section 1.

Reference for Problems 3, 4: Kato, *Perturbation Theory for Linear Operators*, pp. 38–43, Springer-Verlag, Berlin and New York, 1966.

5. Let H_0 be a self-adjoint matrix with eigenvalues $E_0 < E_1 < E_2 < \cdots < E_k$. Suppose that E_0 is a nondegenerate eigenvalue. Let V be an arbitrary self-adjoint matrix and let $E_0 + \sum_{n=1}^{\infty} \alpha_n \beta^n$ be the Rayleigh–Schrödinger series for the eigenvalue of $H_0 + \beta V$ near E_0.
   (a) Prove that all the α_n are real.
   (b) Prove that $\alpha_2 \leq 0$.
   (c) Find an explicit example with $\alpha_4 > 0$.
   (d) If $V \geq 0$ in the sense of matrix inequality, prove that $\alpha_1 \geq 0$.
   (e) Find an explicit example with $V \geq 0$ but $\alpha_3 \leq 0$.

   (Hint for (c) and (e): Use an example of 2×2 matrices and solve the secular equation for 2×2 matrices explicitly.)

†6. (a) Let P be a bounded operator on a Banach space X with $P^2 = P$. Prove that $E = \text{Ran } P$ and $F = \text{Ker } P$ are closed subspaces in X with $E \cap F = \{0\}$ and $E + F = X$. Prove that any $x \in X$ can be uniquely written as $x = e + f$ with $e \in E, f \in F$.
   (b) Conversely, given closed subspaces E and F of a Banach space X with $E \cap F = \{0\}$ and $E + F = X$, prove there is a unique *bounded* operator P on X with $P^2 = P$ and $F = \text{Ker } P$; $E = \text{Ran } P$. (Hint: Use the closed graph theorem.)

7. Prove the following additional fact about the situation described in Theorem XII.6. If $\dim P = n$ and $\nu_1, \ldots, \nu_k$ are the eigenvalues of A in $\{\nu \,|\, |\nu - \lambda| < r\}$, then $\sum_{i=1}^{k} m_i = n$ if m_i is the algebraic multiplicity of ν_i as an eigenvalue.

†8. Let $T(\beta)$ be a family of bounded operators defined on a region $R \subset \mathbb{C}$ so that $\sup_{\beta \in R} \|T(\beta)\| < \infty$. Prove that $T(\beta)$ is an analytic function in the sense of Section VI.3 if and only if $T(\beta)$ is an analytic family in the sense of Kato.

†9. A function F defined on an open set D of a Banach space X taking values in Y, another Banach space, is called analytic if and only if for all $x \in D$, there are functions $f_x^{(1)}, \ldots, f_x^{(n)}, \ldots$ with $f_x^{(j)}$ a j-linear function from $X \times \cdots \times X$ (j times) to Y so that

   (i) For some C and R, $\|f_x^{(j)}(y_1, \ldots, y_j)\| \leq CR^{-j}\|y_i\| \cdots \|y_j\|$.
   (ii) If $\|y\| < R$, $F(x + y) = \sum_{j=0}^{\infty} f_x^{(j)}(y, y, \ldots, y)$ where $f_x^{(0)} = F(x)$.

   (a) Let $\Omega \subset \mathbb{C}$. Let Y be a complex Banach space. Prove that $F : \Omega \to Y$ is analytic in the above sense if and only if it is analytic in the sense of Section VI.3.

(b) If F is an analytic function on $D \subset X$ taking values in Y and if g is an analytic function on a subset Ω of $\mathbb{C}$ taking values in D let $F \circ g: \Omega \to Y$. Prove $F \circ g$ is analytic in the sense of Section VI.3.

(c) Let $X = \mathscr{L}(Z)$ the bounded operators on some Banach space Z. Let $D = \{A \in X \mid A$ has a bounded inverse$\}$. Prove $F(A) = A^{-1}$ is an analytic function on D with values in X.

†*10.* Let $T(\beta)$ be an analytic family of type (A) in a neighborhood of $\beta = 0$.

(a) Prove that there exist operators T_n with $D(T_n) \supset D(T_0)$ and $T_0 \equiv T(0)$ so that (i) For some a, b, and c, and all $\psi \in D(T(0))$: $\|T_n\psi\| \leq c^{n-1}(a\|T(0)\psi\| + b\|\psi\|)$. (ii) For any $\psi \in D(T(0))$ and $|\beta|$ sufficiently small, $T(\beta)\psi = \sum_{n=0}^{\infty} \beta^n T_n \psi$ where the sum is norm convergent.

(b) Prove that a general analytic family of type (A) is an analytic family in the sense of Kato.

Reference for Problem 10: Kato's book (see Problem 4), pp. 375–381.

†*11.* Suppose $V << H_0$, $W << H_0$. Prove that $W << H_0 + V$.

†*12.* In the context of Theorem XII.9, prove that for β small $(H_0 - \lambda)^{-1} \times [1 + \beta V(H_0 - \lambda)^{-1}]^{-1} = A$ is an inverse for $H_0 + \beta V - \lambda$. Explicitly Ran $A \subset D(H_0)$ and $(H_0 + \beta V - \lambda)A\psi = \psi$ for all $\psi \in \mathscr{H}$ and $A(H_0 + \beta V - \lambda)\psi = \psi$ for all $\psi \in D(H_0)$.

13. Let $A(\beta)$ be a compact operator-valued function on a connected open set $R \subset \mathbb{C}$. Let $f(\beta)$ be an analytic function on R. Suppose $f(\beta) \neq 0$ for all $\beta \in R$ and that $f(\beta_i)$ is an eigenvalue of $A(\beta_i)$ for $\beta_1, \ldots, \beta_n, \ldots \in R$ where $\beta_1, \ldots, \beta_n, \ldots$ have a limit point in R. Conclude that $f(\beta)$ is an eigenvalue of $A(\beta)$ for all $\beta \in R$. (Hint: Apply the analytic Fredholm theorem to $f(\beta)^{-1}A(\beta)$.)

†*14.* Prove Theorem XII.11. Reference: Kato's book, pp. 88–89, 379–381.

15. Let $H(\beta)$ be an analytic family in the sense of Kato in a simply connected region $R \subset \mathbb{C}$. Suppose that $E(\beta)$ is an isolated nondegenerate eigenvalue of $H(\beta)$ for each $\beta \in R$. Prove there is an analytic vector valued function ψ on R with $H(\beta)\psi(\beta) = E(\beta)\psi(\beta)$ and $\psi(\beta) \neq 0$ for all $\beta \in R$. (Hint: Use Theorem XII.12.)

16. Suppose that $P_i(\beta)$ is an analytic, projection-valued function of β for all β in R a connected, simply connected region of $\mathbb{C}$, for $i = 1, \ldots, k$. Suppose that $P_i(\beta)P_j(\beta) = 0$ if $i \neq j$ and $\beta \in R$ and $\sum_{i=1}^{k} P_i(\beta) = 1$. Suppose $0 \in R$. Find $U(\beta)$ analytic in R and invertible so that $U(\beta)P_i(0)U(\beta)^{-1} = P_i(\beta)$ for all $\beta \in R$ with $U(\beta)$ unitary for β real if the $P_i(\beta)$ are all orthogonal for β real. (Hint: Mimic the proof of Theorem XII.12 but take $Q(\beta) = \frac{1}{2}\sum_{i=1}^{k} [P_i'(\beta), P_i(\beta)]$.)

17. Let $T(\beta)$ be an analytic $n \times n$ matrix-valued function in a neighborhood of zero. Suppose that $T(\beta)$ is self-adjoint for all real β.

(a) Suppose that E_0 is an eigenvalue of multiplicity m for $T(0)$ and that $E_1(\beta), \ldots, E_k(\beta)$ are the distinct eigenvalues of $T(\beta)$ near E_0. Prove first that the projections $P_i(\beta)$ and $E_i(\beta)$ are meromorphic at $\beta = 0$. Then, using the self-adjointness, prove that the $P_i(\beta)$ are analytic at $\beta = 0$.

(b) Prove that there are analytic vector-valued functions $\psi_1(\beta), \ldots, \psi_n(\beta)$ in a neighborhood of zero so that the $\psi_i(\beta)$ are eigenvectors and $(\psi_i(\beta), \psi_j(\beta)) = \delta_{ij}$ for all real β. (Hint: Use Problem 16.)

†*18.* Complete the proof of the lemma to the proof of Theorem XII.12.

19. Let P and Q be (not necessarily orthogonal) projections on a Hilbert space with $\|P - Q\| < 1$. Let $A = (1 - P)(1 - Q) + PQ$; $B = (1 - Q)(1 - P) + QP$; $C = [1 - (P - Q)^2]$.

(a) Prove that $AB = BA = C$.
(b) Let $\sum_{n=0}^{\infty} \alpha_n x^n$ be the Taylor series for $(1 - x)^{-1/2}$ about $x = 0$ and let $D = \sum_{n=0}^{\alpha} \alpha_n (P - Q)^n$ which converges since $\|P - Q\| < 1$. Prove that $D^2C = CD^2 = DCD = 1$.
(c) Prove that $P(P - Q)^2 = (P - Q)^2 P$ and $Q(P - Q)^2 = (P - Q)^2 Q$. Conclude that $DP = PD$; $QD = DQ$.
(d) Let $W = DA$. Prove W^{-1} exists and $W^{-1} = BD$.
(e) Prove that $WQ = PW$.
(f) If P and Q are self-adjoint, prove that W is unitary.

20. Let $A(\beta)$ be a finite-matrix-valued analytic function defined near $\beta = 0$. Let E_0 be an eigenvalue of $\beta = 0$ of multiplicity m. Let $g_1(\beta), \ldots, g_k(\beta)$ be the multivalued analytic functions defined near $\beta = 0$ whose values are all the eigenvalues of $A(\beta)$ near E_0. Let $P_j(\beta)$ be the eigenprojection

$$(-2\pi i)^{-1} \int_{|\mu - g_j(\beta)| = \varepsilon} (A(\beta) - \mu)^{-1} \, d\mu$$

(a) Prove that $P_j(\beta)$ is multivalued analytic near $\beta = 0$ and that $|\beta|^k \|P_j(\beta)\|$ is bounded as $\beta \to 0$ for some k.
(b) Prove that if $A(\beta)$ is self-adjoint for β real, then $P_j(\beta)$ is single-valued analytic near and at $\beta = 0$.

21. The purpose of this problem is to prove Butler's theorem: If some eigenvalue $g_j(\beta)$ (see Problem 20) is not single valued, then $\|P_j(\beta)\| \to \infty$ as $\beta \to 0$.
(a) Use Problem 20 to prove that if $\|P_j(\beta)\|$ does not diverge, then $P_j(\beta)$ has a Puiseux expansion

$$P_j(\beta) = A_0 + \beta^{1/m} A_1 + \cdots$$

(b) Prove that $A_0^2 = A_0$. (Hint: $P_j(\beta)^2 = P_j(\beta)$.)
(c) Prove that $A_0^2 = 0$. (Hint: $P_j(\beta e^{2\pi i}) P_j(\beta) = 0$.)
(d) Conclude that $P_j(\beta) \to 0$ as $\beta \to 0$.
(e) Prove that any nonzero projection Q obeys $\|Q\| \geq 1$.
(f) Conclude that $\|P_j(\beta)\| \to \infty$.
Reference: Butler's paper quoted in the Notes to Section 1.

22. Use Butler's theorem to prove Rellich's theorem (Theorem XII.3).

23. Let $A(\beta)$ be a finite-matrix-valued analytic function near $\beta = 0$. Suppose that E_0 is an eigenvalue of $A(0)$ with associated eigennilpotent $N \neq 0$ (see Problems 3, 4). Suppose that, for β near 0, the eigenvalues of $A(\beta)$ near E_0 have zero associated eigennilpotents. Prove that the projections $P_j(\beta)$ of Problem 20 have a singularity at $\beta = 0$.

24. Under the hypothesis of Theorem XII.14, prove there is a vector-valued function $\Omega(\beta)$, analytic in the region $\{\beta \,|\, |\arg \beta| < \theta, \ |\beta| < B\}$ for some $B > 0$ so that (i) $H(\beta)\Omega(\beta) = E(\beta)\Omega(\beta)$; (ii) $(\Omega_0, \Omega(\beta)) \equiv 1$; (iii) $\Omega(\beta)$ has an asymptotic series $\sum \varphi_n \beta^n$ as $|\beta| \downarrow 0$; $|\arg \beta| < \theta$, whose terms are given by expressions involving only V, $(H_0 - \lambda)^{-1}$, and Ω_0.

†25. Under the hypotheses of Theorem XII.14, for any vector $\Omega \in C^\infty(H_0)$ and any compact set $K \subset \rho(H_0)$, $[V(H_0 - E)^{-1}]^N\Omega$ is a norm continuous function of E in K. (Hint: Topologize $C^\infty(H_0)$ with the norms $\|\Omega\|_n = \|(|H_0| + 1)^n\Omega\|$. Prove that V is a continuous map from $C^\infty(H_0)$ to itself).

†26. A sequence $(a_0, a_1, \ldots)$ of complex numbers can be thought of as a **formal series** $\sum a_n z^n$. The set of all formal series F supports a sum $(a_0, \ldots) + (b_0, \ldots) = (c_0, \ldots)$ with $c_n = a_n + b_n$ and a multiplication $(a_0, \ldots) \cdot (b_0, \ldots) = (d_0, \ldots)$ with $d_n = \sum_{m=0}^n a_m b_{n-m}$.
(a) Prove that F with these operations is an integral domain with $(1, 0, \ldots)$ as multiplicative identity.
(b) Prove that $(b_0, b_1, \ldots)$ has a multiplicative inverse in F if and only if $b_0 \neq 0$.
(c) Let A and B be formal series with $b_0 \neq 0$. Let C be the formal series $C = AB^{-1}$. Prove that C is the asymptotic series of f/g if A is an asymptotic series for f and B is an asymptotic series for g.
(d) Prove the analogue of (c) with *strong asymptotic* replacing *asymptotic*.

†27. Let A and B be closed operators with $D(A) \cap D(B)$ dense. Prove that $C = A + B$ is closed on $D(A) \cap D(B)$ if and only if $A^*A + B^*B \leq \alpha(C^*C + 1)$ for some constant α.

†28. Using the creation and annihilation operators $A^\dagger$, A of Section V.3, prove the estimates (iii), (iv), (v) in Theorem XII.16 for Example 3 of Section 3.

†29. (a) Prove that any function $g(z)$ analytic in $R = \{z \mid 0 < |z| < B, |\arg z| < k\pi/2 + \varepsilon\}$ with $|g(z)| \leq A\sigma^N[k(N+1)]!\,|z|^N$ for all N and $z \in R$ is identically zero. (Hint: Let $h(w) = g(w^k)$ and apply Theorem XII.18 to h.)
(b) Extend the Borel summability method and Watson's theorem to treat functions f analytic in the region R above obeying a strong asymptotic condition of order k.

30. Let V be given, a closed operator with $C^\infty(H_0) \subset D(V)$ for some self-adjoint operator H_0. Let K be a compact subset of $\rho(H_0)$ and let $H(\beta)$, closed operators, be defined for $0 < |\beta| < B$; $|\arg \beta| \leq \theta$ so that (i) $H(\beta) \restriction C^\infty(H_0) = H_0 + \beta V$. (ii) for $|\beta| < B$, $K \subset \rho(H(\beta))$ for all β. Prove that

$$(H(\beta) - z)^{-1} \underset{\substack{|\beta|\to 0 \\ |\arg\beta|\leq\theta}}{\to} (H_0 - z)^{-1}$$

strongly for all $z \in K$ if and only if for each $z \in K$,

$$\limsup_{\substack{|\beta|\to 0 \\ |\arg\beta|\leq\theta}} \|(H(\beta) - z)^{-1}\| < \infty$$

†31. Let $P^{(n)}$ be a sequence of projection valued measures so that

$$P^{(n)}(a_0 + a_1\beta - f(\beta),\ a_0 + a_1\beta + f(\beta)) \xrightarrow{s} P_\infty$$

and

$$P^{(n)}(b_0 + b_1\beta - g(\beta),\ b_0 + b_1\beta + g(\beta)) \xrightarrow{s} P_\infty$$

where P_∞ is a nonzero projection and $f(\beta)/\beta \to 0$, $g(\beta)/\beta \to 0$. Prove that $a_0 = b_0$ and $a_1 = b_1$. (Hint: $P^{(n)}(\Omega)P^{(n)}(\Omega') = 0$ if $\Omega \cap \Omega' = \varnothing$.)

†32. Under hypotheses (i) and (ii) of Theorem XII.23, prove that
(a) $(H_0 + i)[D(H_0) \cap D(V)]$ is dense in $\mathscr{H}$.
(b) $(H_0 + i)^{-1} - (H_0 + \beta V + i)^{-1} \to 0$ strongly as $\beta \to 0$.

†33. Prove the formula

$$a_2 = (2\pi i)^{-1} \oint_{|E - E_0| = \varepsilon} (\overline{\Omega(\theta; 0)}, V[H_0(\theta) - E]^{-1} V\Omega(\theta; 0)) \frac{dE}{E - E_0}$$

for the situation described in Section 6. (Hint: Use the methods of Section 1 taking into account that $H_0(\theta)$ is not self-adjoint but that $H_0^*(\theta)\overline{f} = \overline{H_0(\theta)f}$.)

†34. Consider the situation described in Section 6 where $H(\theta)$ is an analytic family in θ with $H(\theta) = U(\theta)HU(\theta)^{-1}$ for θ real and

$$\sigma_{ess}(H(\theta)) = \{\lambda + xe^{-2\theta} \mid \lambda \in \sum; x \in \mathbb{R}_+\}$$

with $\sum = \{-1/n^2\}$. Suppose that $H(\theta)$ has a real eigenvalue $E_0 \notin \sum$ for all θ with $\operatorname{Im} \theta > 0$. Write $H(0) \equiv H$.
(a) Find vectors $\psi \in \mathscr{H}$ so that $(\psi, (H - z)^{-1}\psi)$ has an analytic continuation below the real axis near E_0 with a pole at E_0 with nonzero residue.
(b) For $\psi \in \mathscr{H}$, prove that $\lim_{\varepsilon \downarrow 0} (z - E_0)(\psi, (H - z)^{-1}\psi)|_{z = E_0 + i\varepsilon} \neq 0$.
(c) For any self-adjoint operator A, prove that

$$\text{s-}\lim_{\varepsilon \downarrow 0} (z - E_0)(A - z)^{-1} \Big|_{z = E_0 + i\varepsilon} = P_{\{E_0\}},$$

the spectral projection onto the point E_0. (Hint: Use the functional calculus.)
(d) Conclude that E_0 is an eigenvalue of H.
(e) Prove that $(\psi, (H - z)^{-1}\psi)$ cannot have a double pole at E_0 for any $\psi \in \mathscr{H}$.
(f) Let $\varphi = P(\theta)\varphi$ for some θ with $\operatorname{Im} \theta > 0$, where

$$P(\theta) = -(2\pi i)^{-1} \oint_{|E - E_0| = \varepsilon(\theta)} (H(\theta) - E)^{-1}\, dE.$$

Prove that $H(\theta)\varphi = E_0\varphi$.
Remark: In general, following Problem 4, $(H(\theta) - E_0)^n\varphi = 0$ for some n, but using (e), (f) can be proven.
(g) Prove $\dim \operatorname{Ran}(P(\theta)) = \dim \operatorname{Ran}(P_{\{E_0\}})$.
(h) If E_0' is an eigenvalue of H, prove it is an eigenvalue of $H(\theta)$ if $\operatorname{Im} \theta > 0$.

†35. Under the conditions of Problem 34,
*(a) Prove that $P(\theta) \to P_{\{E_0\}}$ strongly as $\theta \to 0$ with $\operatorname{Im} \theta > 0$.
(b) Prove that $P(\theta)$ extends to a function analytic in a strip $|\operatorname{Im} \theta| \leq b$. (Hint: Use the Schwarz reflection principle.)
(c) For θ real, prove that $P(\theta) = U(\theta)P_{\{E_0\}}U(\theta)^{-1}$.
(d) For $\Omega_0 \in \operatorname{Ran} P_{\{E_0\}}$, prove that $U(\theta)\Omega_0$ has an analytic continuation to a strip $|\operatorname{Im} \theta| \leq b$ with $U(\theta)\Omega_0 \in D(H(\theta))$ for all θ.

Reference for Problems 34 and 35: The Balslev–Combes article mentioned in the Notes to Section XIII.10.

†36. Fill in the details of Example 6 of Section 3.

XIII: Spectral Analysis

If an atom can vibrate in more ways than one, it is certain that some connection must exist between the different periods, and this connection we may attempt to find out by trial. Or we may speculate on the causes which produce such vast differences in the chemical properties of some of the elements, while other elements have properties which resemble each other to an equally marked degree. We may be led on by such speculations to try whether we can trace any similarity in the periods of vibration of molecules which have similar chemical properties, or we may endeavour to classify the elements according to their spectra, and see whether such a classification would divide the elements into groups agreeing with those into which they have been divided by means of their chemical and physical behaviour.

A. Schuster, 1882

XIII.1 The min–max principle

In this chapter we describe methods for determining the spectral properties of a given self-adjoint operator H. We want information not only about the spectrum of H, $\sigma(H)$, but also about the subsets $\sigma_{\text{ess}}(H)$, $\sigma_{\text{disc}}(H)$, $\sigma_{\text{ac}}(H)$, $\sigma_{\text{sing}}(H)$, $\sigma_{\text{pp}}(H)$ defined in Sections VII.2 and VII.3. We are interested in quantitative information such as a precise determination of some or all of these subsets, and in qualitative information such as "$\sigma_{\text{disc}}(H)$ is finite" or "$\sigma_{\text{pp}} \subset (\sigma_{\text{disc}} \cup \partial\sigma_{\text{ess}})$."

In this section we shall develop a method for obtaining information about $\sigma_{\text{disc}}(H)$ and $\sigma_{\text{ess}}(H)$ from knowledge of the expectation values $(\psi, H\psi)$. This method is especially useful in the case that H has essential spectrum $[a, \infty)$ for some $a > -\infty$ and some eigenvalues in $(-\infty, a)$. This is the usual case encountered for Hamiltonians in quantum theories.

To understand the sort of result we would like, suppose that A and B are two 3×3 self-adjoint matrices with $A \leq B$ in the sense that $(\psi, A\psi) \leq (\psi, B\psi)$ for all $\psi \in \mathbb{C}^3$. Let $\lambda_1(A), \lambda_2(A), \lambda_3(A)$ be the three eigenvalues of A, listed so that $\lambda_1(A) \leq \lambda_2(A) \leq \lambda_3(A)$, and similarly for $\lambda_i(B)$, $i = 1, 2, 3$. Since $A \leq B$, we expect $\lambda_i(A) \leq \lambda_i(B)$ for $i = 1, 2, 3$. Can we prove this? Let $\psi_1, \psi_2,$

ψ_3 be the three eigenvectors of A chosen to be orthonormal. Writing $\psi = \alpha_1\psi_1 + \alpha_2\psi_2 + \alpha_3\psi_3$, we see that

$$\frac{(\psi, A\psi)}{(\psi, \psi)} = \frac{|\alpha_1|^2\lambda_1(A) + |\alpha_2|^2\lambda_2(A) + |\alpha_3|^2\lambda_3(A)}{|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2}$$

so $\lambda_1(A) = \min_{\psi\neq 0}(\psi, A\psi)/(\psi, \psi)$ and $\lambda_3(A) = \max_{\psi\neq 0}(\psi, A\psi)/(\psi, \psi)$. These formulas and the similar formulas for $\lambda_1(B)$, $\lambda_3(B)$ imply $\lambda_1(A) \leq \lambda_1(B)$ and $\lambda_3(A) \leq \lambda_3(B)$ if $A \leq B$. What remains is to show that $\lambda_2(A) \leq \lambda_2(B)$. So we seek a formula for $\lambda_2(A)$ similar to our formula for $\lambda_1(A)$ in terms of $(\psi, A\psi)$. First, note that

$$\lambda_2 = \min_{\substack{\{\alpha_1,\alpha_2,\alpha_3\}\neq 0\\ \alpha_1=0}} \frac{\alpha_1^2\lambda_1 + \alpha_2^2\lambda_2 + \alpha_3^2\lambda_3}{\alpha_1^2 + \alpha_2^2 + \alpha_3^2}$$

or equivalently,

$$\lambda_2(A) = U_A(\psi_1)$$

where

$$U_A(\psi) = \min_{\{\varphi \mid (\varphi,\psi)=0,\ \varphi\neq 0\}} (\varphi, A\varphi)/(\varphi, \varphi)$$

This is not quite of the required form since $U_A(\psi_1)$ depends not only on $(\varphi, A\varphi)$ for all φ but on ψ_1. But, notice that for arbitrary ψ, we can find some $\varphi = \alpha_1\psi_1 + \alpha_2\psi_2$ with $\langle\alpha_1, \alpha_2\rangle \neq \langle 0, 0\rangle$ which is orthogonal to ψ. Thus there is a φ with $(\varphi, \psi) = 0$ and $(\varphi, A\varphi)/(\varphi, \varphi) \leq \lambda_2(A)$. So, for all ψ, $U_A(\psi) \leq \lambda_2(A)$. We conclude that

$$\lambda_2(A) = \max_{\psi} \min_{\substack{\varphi\in[\psi]^\perp\\ \varphi\neq 0}} (\varphi, A\varphi)/(\varphi, \varphi) \tag{1}$$

This expresses $\lambda_2(A)$ in terms of $(\varphi, A\varphi)$ only and can be used to prove $\lambda_2(A) \leq \lambda_2(B)$ (Problem 1).

We are now interested in extending (1) to the nth eigenvalue of a self-adjoint operator on an infinite-dimensional space. There are two problems: (1) the occurrence of nonpoint spectrum; (2) domain questions. These problems are overcome by a careful statement of the main result of this section:

Theorem XIII.1 (min–max principle, operator form) Let H be a self-adjoint operator that is bounded from below, i.e., $H \geq cI$ for some c. Define

$$\mu_n(H) = \sup_{\varphi_1,\ldots,\varphi_{n-1}} U_H(\varphi_1, \ldots, \varphi_{n-1})$$

where

$$U_H(\varphi_1, \ldots, \varphi_m) = \inf_{\substack{\psi \in D(H);\ \|\psi\| = 1 \\ \psi \in [\varphi_1, \ldots, \varphi_m]^\perp}} (\psi, H\psi)$$

$[\varphi_1, \ldots, \varphi_m]^\perp$ is shorthand for $\{\psi \,|\, (\psi, \varphi_i) = 0,\ i = 1, \ldots, m\}$. Note that the φ_i are not necessarily independent.

Then, for each fixed n, *either*:

(a) there are n eigenvalues (counting degenerate eigenvalues a number of times equal to their multiplicity) below the bottom of the essential spectrum, and $\mu_n(H)$ is the nth eigenvalue counting multiplicity;

or

(b) μ_n is the bottom of the essential spectrum, i.e., $\mu_n = \inf\{\lambda \,|\, \lambda \in \sigma_{\text{ess}}(H)\}$ and in that case $\mu_n = \mu_{n+1} = \mu_{n+2} = \cdots$ and there are at most $n - 1$ eigenvalues (counting multiplicity) below μ_n.

Proof Let P_Ω be the projection-valued measure for H. We first prove that

$$\dim[\text{Ran}(P_{(-\infty, a)})] < n \qquad \text{if} \quad a < \mu_n \tag{2a}$$

$$\dim[\text{Ran}(P_{(-\infty, a)})] \geq n \qquad \text{if} \quad a > \mu_n \tag{2b}$$

For suppose (2a) is false. Then we can find an n-dimensional space $V \subset D(H)$ so that for any $\psi \in V$, $(\psi, H\psi) \leq a\|\psi\|^2$. That $V \subset D(H)$ is a consequence of the fact that H is bounded from below, which implies that $\text{Ran}(P_{(-\infty, a)}) \subset D(H)$ if $a < \infty$. But then given any $\varphi_1, \ldots, \varphi_{n-1}$, we can find $\psi \in V \cap [\varphi_1, \ldots, \varphi_{n-1}]^\perp$. Thus $U(\varphi_1, \ldots, \varphi_{n-1}) \leq a$ for any $\varphi_1, \ldots, \varphi_{n-1}$ so $\mu_n(H) \leq a$ contradicting the basic hypothesis. This proves (2a).

Next, suppose that (2b) is false. Then $\dim(\text{Ran}(P_{(-\infty, a)})) \leq n - 1$, so we can find $\varphi_1^{(0)}, \ldots, \varphi_{n-1}^{(0)}$ with $[\varphi_1^{(0)}, \ldots, \varphi_{n-1}^{(0)}] = \text{Ran}(P_{(-\infty, a)})$. Then any $\psi \in [\varphi_1^{(0)}, \ldots, \varphi_{n-1}^{(0)}]^\perp \cap D(H)$ is in Ran $P_{[a, \infty)}$, so $(\psi, H\psi) \geq a\|\psi\|^2$. Therefore, $U(\varphi_1^{(0)}, \ldots, \varphi_{n-1}^{(0)}) \geq a$ and $\mu_n \geq a$, contradicting the basic hypothesis. This proves (2b).

Notice that (2) and the fact that H is bounded from below imply that μ_n is finite. There are two distinct cases to consider:

Case 1 $\dim(\text{Ran } P_{(-\infty, \mu_n + \varepsilon)}) = \infty$ for all $\varepsilon > 0$. We claim we are then in the situation described by (b) in the theorem. For, by (2a), $\dim(\text{Ran } P_{(-\infty, \mu_n - \varepsilon]}) \leq n - 1$ and therefore $\dim P_{(\mu_n - \varepsilon, \mu_n + \varepsilon)} = \infty$ for all $\varepsilon > 0$. By the definition of σ_{ess}, $\mu_n \in \sigma_{\text{ess}}(H)$. On the other hand, again using (2a), if $a < \mu_n$ and $0 < \varepsilon < \mu_n - a$, then $\dim P_{(a - \varepsilon, a + \varepsilon)} < n < \infty$, so $a \notin \sigma_{\text{ess}}(H)$. Thus $\mu_n = \inf\{\lambda \,|\, \lambda \in \sigma_{\text{ess}}(H)\}$. Next notice that in general

$\mu_{n+1} \geq \mu_n$ since one can take $\varphi_{n+1} = \varphi_n$. Therefore $\mu_{n+1} = \mu_n$ for if $\mu_{n+1} > \mu_n$, then dim $P_{(-\infty, \frac{1}{2}\mu_n + \frac{1}{2}\mu_{n+1})} \leq n$ by (2a), contradicting the hypothesis that dim $P_{(-\infty, \mu_n + \varepsilon)} = \infty$. Finally, we note that if there were n eigenvalues strictly below μ_n, and a were the nth eigenvalue, then dim $P_{(-\infty, \frac{1}{2}a + \frac{1}{2}\mu_n)} \geq n$, contradicting (2a). Thus the situation in (b) holds.

Case 2 dim $P_{(-\infty, \mu_n + \varepsilon_0)} < \infty$ for some $\varepsilon_0 > 0$. We claim we are then in the situation described by (a) in the theorem. For by (2), dim $P_{(\mu_n - \varepsilon, \mu_n + \varepsilon)} \geq 1$ for all ε, so $\mu_n \in \sigma(H)$ by the proposition in Section VII.3. But dim $P_{(\mu_n - \varepsilon_0, \mu_n + \varepsilon_0)} < \infty$, so $\mu_n \in \sigma_{\text{disc}}(H)$ by definition. Therefore, μ_n is an eigenvalue and we can find δ with $(\mu_n - \delta, \mu_n + \delta) \cap \sigma(H) = \{\mu_n\}$. Then dim $P_{(-\infty, \mu_n]} = \dim P_{(-\infty, \mu_n + \delta)} \geq n$, so there are at least n eigenvalues $E_1 \leq \cdots \leq E_n \leq \mu_n$. If E_n were less than μ_n, then dim $P_{(-\infty, E_n)}$ would equal n, violating (2a). Thus $E_n = \mu_n$, i.e., μ_n is the nth eigenvalue. This shows we are in situation (a). ∎

There is another formulation of the min–max principle which differs on one technical point and which is also useful:

Theorem XIII.2 If H is self-adjoint and bounded from below, then

$$\mu_n = \sup_{\varphi_1, \ldots, \varphi_{n-1}} \inf_{\substack{\psi \in [\varphi_1, \ldots, \varphi_{n-1}]^\perp \\ \|\psi\| = 1;\, \psi \in Q(H)}} (\psi, H\psi) \tag{3}$$

where $Q(H)$ is the form domain of H.

Proof Let $\tilde{\mu}_n$ denote the right-hand side of (3). By mimicking the proof of Theorem XIII.1, we can prove that each $\tilde{\mu}_n$ obeys either condition (a) or condition (b) of Theorem XIII.1. These conditions determine the μ_n, so $\tilde{\mu}_n = \mu_n$. ∎

We shall turn to applications of the min–max principle in the next three sections. Let us however make a few general remarks:

(1) As we saw in our motivating example, the min–max principle is ideal for comparing eigenvalues of operators. This can have both quantitative and qualitative consequences.

(2) The method can be useful in locating where σ_{ess} begins. In particular, we shall see it tells us that σ_{ess} is empty in some cases (see Sections 4 and 14).

(3) In Sections 4 and 5, we shall prove that in certain cases $\sigma_{\text{ess}}(H) = [a, \infty)$ for explicit a. Suppose we know in addition that $\mu_n < a$. Then we can conclude that H has at least n eigenvalues! Thus the min–max principle can be used to prove the existence of discrete spectrum in some situations.

The following proposition shows how the min–max principle can be applied.

Proposition Let $A \geq 0$ and B be self-adjoint operators. Suppose that $Q(A) \cap Q(B)$ is dense and that B_-, the negative part of B, is relatively form bounded with respect to A with relative bound zero. For $\beta \geq 0$, let $A + \beta B$ denote the operator associated to the obvious form sum. Suppose that $\sigma_{\text{ess}}(A + \beta B) = [0, \infty)$ for all $\beta \geq 0$. Then $\mu_n(A + \beta B)$ is monotone nonincreasing on $[0, \infty)$.

Proof Since $\mu_n(A + \beta B) \leq 0$ for all n, by the hypothesis on $\sigma_{\text{ess}}(A + \beta B)$, we have

$$\mu_n(A + \beta B) = \max_{\varphi_1, \ldots, \varphi_{n-1}} \min_{\substack{\psi \in Q(A) \cap Q(B) \\ \|\psi\| = 1,\ \psi \in [\varphi_1, \ldots, \varphi_{n-1}]^\perp}} [\min\{0, (\psi, (A + \beta B)\psi)\}]$$

Since $A \geq 0$, it is easy to see that $\min\{0, (\psi, (A + \beta B)\psi)\}$ is monotone nonincreasing in β. ∎

Example In Section 4, we shall prove that $\sigma_{\text{ess}}(-\Delta + \beta V) = [0, \infty)$ for a wide class of V's. The proposition shows that for such V's the negative eigenvalues and, in particular, $\inf \sigma(-\Delta + \beta V)$ are monotone decreasing in β and that the number of negative eigenvalues is monotone increasing.

XIII.2 Bound states of Schrödinger operators I: Quantitative methods

The min–max principle is useful for studying a wide variety of aspects of the point spectrum. In this section and the next we shall describe properties of the discrete spectrum of operators of the form $-\Delta + V$, the Hamiltonians of nonrelativistic quantum mechanics. These operators are often called **Schrödinger operators** and the eigenvectors associated to the discrete spectrum are called **bound states**. Points in the discrete spectrum are called **bound state energies** (or **energy levels**). In this section we develop the Rayleigh–Ritz technique for finding bound state energies to very high accuracy. In the next section we concentrate on qualitative aspects of the spectrum. Readers primarily interested in the min–max principle should read this section and the first part of the next.

The Hamiltonian of the elementary model for the helium atom is

$$H = -\Delta_1 - \Delta_2 - \frac{2}{|r_1|} - \frac{2}{|r_2|} + \frac{1}{|r_1 - r_2|}$$

on $L^2(\mathbb{R}^6)$. We have used atomic units, i.e., units with $\hbar = e^2 = 2\mu_e = 1$ where μ_e is the reduced mass of an electron–helium nucleus system. Unlike the hydrogen atom model, it is not possible to solve exactly the eigenvalue problem $H\psi = E\psi$. We wish to describe here methods for finding the lowest eigenvalue of H to high accuracy, but first we should like to explain the physical interest in this eigenvalue. The method also allows one to approximate higher eigenvalues.

The energy needed to ionize the helium atom can be measured. In the simplest model this ionization energy is just the difference between the lowest eigenvalue of H and the ground state energy of a helium ion. In the model the latter quantity is exactly calculable since it is related to the exactly soluble one-body Coulomb problem. In the early days of quantum theory, "crude" agreement (i.e., to about 0.01%) between this model computation and the measured ionization energy was an important experimental confirmation of quantum mechanics.

If one wants to compare experiment and theory to higher accuracy, it is necessary to deal with a more sophisticated model Hamiltonian than H. Since the electron spin becomes significant, it is necessary to use $L^2(\mathbb{R}^6) \otimes \mathbb{C}^4$ as the underlying Hilbert space where $\mathbb{C}^4 = \mathbb{C}^2 \otimes \mathbb{C}^2$ describes the spin of the two electrons. We denote $H \otimes I$ as H. The difference between H and the more sophisticated Hamiltonian is in several pieces, each called a correction. Below we shall briefly describe the physical basis for each of these corrections. Each of them has associated with it an operator A_α so that in the more complicated model the Hamiltonian is $H + \sum A_\alpha$. While we shall not be explicit about the form of the A_α, there are well-tested physical theories that lead to explicit operator corrections (see the Notes for references). The operator corrections are:

(1) *The **Hughes–Eckart** term described in Section XI.5.* The fractional change in the lowest eigenvalue due to this correction should be of order m_e/m_α where m_e is the mass of the electron and m_α is the mass of the helium nucleus. This number is about 1.3×10^{-4}.

(2) *The fine structure corrections* These are certain simple relativistic corrections: the **Sommerfeld correction** which is the difference between the relativistic kinetic energy $\sqrt{(m_e c^2)^2 + (pc)^2} - m_e c^2$ and the nonrelativistic kinetic energy $\frac{1}{2}p^2/m_e$; the **spin–orbit** correction which arises physically from the fact that the electron has a magnetic moment that interacts with the

magnetic field set up by the current the electron sees due to the motion of the nucleus relative to it; the **Darwin correction** which arises physically from the fact that a relativistic electron cannot be localized in regions smaller than $\hbar/mc$, so that the electron interacts not with $V(r)$ but an average of $V(r)$ over a sphere of radius approximately $\hbar/mc$; the **retardation term** which is due to the fact that electron one does not feel a force $\text{grad}_1 |r_1 - r_2|^{-1}$ with r_2 the instantaneous position of the second electron but rather due to the finiteness of the speed of light, it feels the force produced by an electron at the position electron two occupied slightly in the past; the **spin–spin** interaction caused by the interactions of the magnetic moments of the electrons. The spin–orbit and spin–spin corrections can be interpreted as relativistic corrections since the magnetic moment of the electron is a relativistic effect. These relativistic corrections are of order $(e^2/\hbar c)^2 \sim 5 \times 10^{-5}$.

Let us suppose that we knew the lowest eigenvalue E of H and the corresponding eigenfunction. Since the correction term $\sum A_\alpha$ is explicitly known, we could attempt to estimate the shift in the lowest eigenvalue by using low-order perturbation theory. In first order each A_α makes a separate contribution. In higher order there are cross terms, but these are smaller than the accuracy of the computations we shall discuss below. It is thus possible to estimate the shift in E due to $\sum A_\alpha$ as a sum of terms associated to each α. We emphasize that the usual form taken for the A_α is sufficiently singular so that the convergence theorems of Chapter XII are not applicable; in fact it is not known that $H + \sum A_\alpha$ is essentially self-adjoint! As a result, these computations are not on a rigorous footing. This problem could be partly eliminated by replacing a delta function nuclear charge distribution with a C^∞ charge distribution strongly peaked near the origin.

In addition to these operator corrections, there is believed to be a shift in the ionization energy due to interactions with the quantized electromagnetic field. This **Lamb shift** can be computed within the framework of the theory of quantum electrodynamics (QED). This theory does not lead to simple operator corrections to H but it does allow approximate calculations of the shift that is predicted to be about one-millionth of the simple model ionization energy.

Quantum electrodynamics is a theory whose internal structure is not completely understood and which is testable in a limited number of experiments. The physicist thus views the ionization energy of helium as a piece of raw data on which to test QED. Since the Lamb shift is only of order 10^{-6}, the experimental data must be obtained to high accuracy, and the other contributions to the ionization energy must be *computed* to great accuracy. Despite the questions of rigor in the perturbation theory calculation of the

shifts due to the A_α, the physicist is willing to accept the predictions of Rayleigh–Schrödinger theory.

The main theoretical problem is then to compute the lowest eigenvalue of H to eight-place accuracy! One might try to start with the exactly soluble operator $-\Delta_1 - 2|r_1|^{-1} - \Delta_2 - 2|r_2|^{-1}$ and treat $|r_1 - r_2|^{-1}$ as a perturbation. In Section XII.2, we saw that the first-order term in the series disagreed with experiment by 15%. Since all the corrections contribute less than 1% to the shift, E presumably differs from first-order perturbation theory by over 10%. To hope to get a numerical answer to one part in 10^8 using perturbation theory is thus effectively impossible. However, one can compute E using a technique suggested by the min–max principle:

Theorem XIII.3 (the Rayleigh–Ritz technique) Let H be a semibounded self-adjoint operator. Let V be an n-dimensional subspace, $V \subset D(H)$, and let P be the orthogonal projection onto V. Let $H_V = PHP$. Let $\hat{\mu}_1, \ldots, \hat{\mu}_n$ be the eigenvalues of $H_V \restriction V$, ordered by $\hat{\mu}_1 \leq \hat{\mu}_2 \leq \cdots \leq \hat{\mu}_n$. Then

$$\mu_m(H) \leq \hat{\mu}_m, \qquad m = 1, \ldots, n$$

In particular, if H has eigenvalues (counting multiplicity) $E_1, \ldots, E_k$ at the bottom of its spectrum with $E_1 \leq \cdots \leq E_k$, then

$$E_m \leq \hat{\mu}_m, \qquad m = 1, \ldots, \min(k, n)$$

Proof By the min–max principle, $H_V \restriction V$ has eigenvalues given by

$$\begin{aligned}
\hat{\mu}_m &= \sup_{\varphi_1, \ldots, \varphi_{m-1} \in V} \inf_{\substack{\psi \in V;\ \|\psi\| = 1 \\ \psi \in [\varphi_1, \ldots, \varphi_{m-1}]^\perp}} (\psi, H\psi) \\
&= \sup_{\varphi_1, \ldots, \varphi_{m-1} \in \mathscr{H}} \inf_{\substack{\psi \in V;\ \|\psi\| = 1 \\ \psi \in [P\varphi_1, \ldots, P\varphi_{m-1}]^\perp}} (\psi, H\psi) \\
&= \sup_{\varphi_1, \ldots, \varphi_{m-1} \in \mathscr{H}} \inf_{\substack{\psi \in V;\ \|\psi\| = 1 \\ \psi \in [\varphi_1, \ldots, \varphi_{m-1}]^\perp}} (\psi, H\psi) \\
&\geq \sup_{\varphi_1, \ldots, \varphi_{m-1} \in \mathscr{H}} \inf_{\substack{\psi \in D(H);\ \|\psi\| = 1 \\ \psi \in [\varphi_1, \ldots, \varphi_{m-1}]^\perp}} (\psi, H\psi) \\
&= \mu_m(H)
\end{aligned}$$

In the third step we used the fact that for $\psi \in V$, $(\psi, P\varphi) = (\psi, \varphi)$. ∎

Thus, to obtain upper bounds on the eigenvalues, and in particular on the lowest eigenvalue E_1, we pick an orthonormal set $\eta_1, \ldots, \eta_n \in D(H)$ and diagonalize the $n \times n$ matrix $(\eta_i, H\eta_j)$ on a computer. Before discussing the

application of this method to the helium atom, let us consider two natural fundamental questions:

(i) We take an orthonormal basis $\{\eta_i\}_{i=1}^{\infty}$ and obtain an upper bound $\hat{\mu}_1^{(n)}$ on E_1 by diagonalizing $\{(\eta_i, H\eta_j)\}_{1 \le i,\, j \le n}$. Does $\hat{\mu}_1^{(n)}$ converge to E_1 as $n \to \infty$?

(ii) Is there any way of obtaining lower bounds on eigenvalues so that one can determine the accuracy of the upper bound?

To answer question (i), we note:

Theorem XIII.4 Let $\{\eta_i\}_{i=1}^{\infty}$ be an orthonormal basis for $\mathscr{H}$ with each $\eta_i \in D(H)$, the domain of a semibounded self-adjoint operator H. Suppose that $\mu_1(H)$ is an eigenvalue E_1 of H with a normalized eigenvector $\psi = \sum_{i=1}^{\infty} a_i \eta_i$. Suppose that

$$\lim_{N \to \infty} \left(\sum_{i=1}^{N} a_i \eta_i \,,\, H\left(\sum_{i=1}^{N} a_i \eta_i \right) \right) = \mu_1(H)$$

Then $\hat{\mu}_1^{(n)} \to E_1$, where $\hat{\mu}_1^{(n)}$ is the lowest eigenvalue of $\{(\eta_i, H\eta_j)\}_{1 \le i,\, j \le n}$.

Proof See Problem 3.

The importance of this theorem is that the convergence of $\lim_{N \to \infty} (\sum_{i=1}^{N} a_i \eta_i,\ H(\sum_{i=1}^{N} a_i \eta_i))$ to $\mu_1(H) = (\psi, H\psi)$ can sometimes be proven on abstract grounds. For example, it always holds if H is bounded since $\sum_{i=1}^{N} a_i \eta_i \to \psi$ in norm. The method needed to prove convergence in case H is not bounded is nicely illustrated by:

Example 1 Suppose that $H = H_0 + V$ with $V \in L^2(\mathbb{R}^3) + (L^\infty(\mathbb{R}^3))_\varepsilon$ and that $\mu_1(H) < 0$. Then one knows that $\mu_1(H)$ is an eigenvalue (see Section 4) which is nondegenerate (see Section 12) and that the corresponding eigenfunction is contained in $D(|x|^2)$ (see Section 11). Since $\psi \in D(H_0)$, $\psi \in D(H_0 + x^2) = D(H_0) \cap D(x^2)$. Let $\{\varphi_i\}$ be the eigenfunctions of the three-dimensional harmonic oscillator (see the Appendix to Section V.3). Then,

$$\lim_{N \to \infty} \left(\left(\sum_{i=1}^{N} a_i \varphi_i - \psi \right), (H_0 + x^2) \left(\sum_{i=1}^{N} a_i \varphi_i - \psi \right) \right) = 0$$

But since $V \in L^2 + L^\infty$, $|V| \le H_0 + b$ for suitable b so

$$H_0 + |V| \le 2H_0 + b \le 2(H_0 + x^2) + b$$

Therefore,

$$\lim_{N\to\infty}\left(\left(\sum_{i=1}^{N}a_i\varphi_i-\psi\right),(H_0+V)\left(\sum_{i=1}^{N}a_i\varphi_i-\psi\right)\right)=0$$

which implies

$$\lim_{N\to\infty}\left(\sum_{i=1}^{N}a_i\varphi_i\,,(H_0+V)\sum_{i=1}^{N}a_i\varphi_i\right)=\mu_1$$

By Theorem XIII.4, $\hat{\mu}_1^{(n)}\to\mu_1$.

Example 2 Let $H=p^2+x^2+\beta x^4$ on $L^2(\mathbb{R})$ where $\beta>0$. Let φ_i be the eigenfunctions of the harmonic oscillator and let ψ be the lowest eigenvector of H. Let $\psi=\sum_{i=1}^{\infty}a_i\varphi_i$. From the form estimates

$$0\le(p^2+x^2+\beta x^4)\le C_1(p^2+x^2)^2\le C_2(p^2+x^2+\beta x^4)^2$$

one can show that

$$\lim_{N\to\infty}\left(\sum_{i=1}^{N}a_i\varphi_i\,,H\sum_{i=1}^{N}a_i\varphi_i\right)=\mu_1(H)$$

so again $\hat{\mu}_1^{(n)}\to\mu_1$. The details are left to the reader as Problem 4.

Notice that it is not really necessary that $\{\eta_i\}_{i=1}^{\infty}$ be an orthonormal basis. What is important is that the ground state eigenvector ψ be in the space generated by the $\{\eta_i\}_{i=1}^{\infty}$ and that the convergence hypothesis in Theorem XIII.4 holds. The use of symmetries and this remark often allow one to simplify computations. For instance, in Example 2 above ψ is an even function of x and so $\psi=\sum_{i=1}^{\infty}a_{2i-1}\varphi_{2i-1}$ and we need only diagonalize $\{(\varphi_{2i-1},H\varphi_{2j-1})\}_{1\le i,\,j\le N}$ to estimate $\mu_1(H)$ or any $\mu_{2k+1}(H)$.

The second question raised above is more interesting. There are several different lower bound techniques; we discuss the simplest one here and mention others briefly in the Notes.

Theorem XIII.5 (Temple's inequality) Let H be a self-adjoint operator that is bounded from below. Suppose that $\mu_1<\mu_2$ and $(\psi,H\psi)<\breve{\mu}_2$ where $\psi\in D(H)$, $\|\psi\|=1$ and $\breve{\mu}_2$ is some number less than μ_2. Then

$$\mu_1\ge(\psi,H\psi)-\frac{(\psi,H^2\psi)-(\psi,H\psi)^2}{\breve{\mu}_2-(\psi,H\psi)}$$

Proof Since μ_1 is a discrete eigenvalue and $\sigma(H)\backslash\{\mu_1\} \subset [\check{\mu}_2, \infty)$, we have $(H - \mu_1)(H - \check{\mu}_2) \geq 0$. Thus,

$$(\psi, (H - \check{\mu}_2)H\psi) \geq \mu_1(\psi, (H - \check{\mu}_2)\psi)$$

By hypothesis, $(\psi, (H - \check{\mu}_2)\psi) < 0$, so

$$\mu_1 \geq \frac{\check{\mu}_2(\psi, H\psi) - (\psi, H^2\psi)}{\check{\mu}_2 - (\psi, H\psi)} = (\psi, H\psi) - \frac{(\psi, H^2\psi) - (\psi, H\psi)^2}{\check{\mu}_2 - (\psi, H\psi)} \quad \blacksquare$$

Notice that the lower bound for μ_1 given by Temple's inequality is close to the upper bound given by Rayleigh–Ritz if ψ is "almost" an eigenvector in the sense that $(\psi, (H - \langle H\rangle)^2\psi)$ is small where $\langle H\rangle = (\psi, H\psi)$.

Temple's inequality requires as input a crude lower bound on the second eigenvalue. This can often be achieved as follows.

Definition Let A and B be self-adjoint operators that are bounded from below. Then we say $A \leq B$ if and only if $Q(B) \subset Q(A)$ and $(\varphi, A\varphi) \leq (\varphi, B\varphi)$ for all φ in $Q(B)$.

The reader is asked in Problem 1 to prove that if $A \leq B$, then $\mu_n(A) \leq \mu_n(B)$.

Example 3 Let H be the helium atom Hamiltonian and let

$$A = -\Delta_1 - \Delta_2 - \frac{2}{|r_1|} - \frac{2}{|r_2|}$$

Then $A \leq H$, so $\mu_2(H) \geq \mu_2(A) = -\frac{5}{4}$.

The application of the Rayleigh–Ritz method to the ground state of helium goes back to the earliest days of quantum theory when Hylleraas made a simple variational Rayleigh–Ritz calculation by hand. In those days the calculation was made as support for elementary quantum mechanics and a calculation with $n = 6$ was sufficient. With the advent of high-speed computers and the need for an accurate computation of $\mu_1(H)$ to test the Lamb shift, more elaborate calculations were needed. An early calculation involving the diagonalization of a 39×39 matrix was made by Kinoshita and one with 1078 parameters by Perkeris! Perkeris' results are summarized by the accompanying tabulation.

Contributions to the Ionization Energy (in units of cm^{-1})	
ΔE (purely Coulombic model)	198 317.374
Hughes–Eckart shift	−4.785
Relativistic corrections	−0.562
Lamb shift theory	-1.351 ± 0.02
Theoretical value	$198\,310.676 \pm 0.02$
Experimental value	$198\,310.82 \pm 0.15$

The error listed for the Lamb shift represents uncertainties in the calculations and mild disagreements between the calculations of various authors. We note that Temple's inequality gives an *upper* bound for $\Delta E = E_{\text{ion}} - E_{\text{atom}}$ of 198 317.866.

We thus see that to within experimental error the Lamb shift agrees with experiment to 1%. This verification of a QED prediction would have been impossible without the accurate calculation of the lowest eigenvalue made possible by the Rayleigh–Ritz method.

XIII.3 Bound states of Schrödinger operators II: Qualitative theory

In this section we discuss certain qualitative features of $N(V)$, the number of bound states of $-\Delta + V$ counting multiplicity. In the first part we investigate whether $N(V)$ is finite or infinite. In the latter parts we obtain bounds on $N(V)$. The min–max principle is used throughout, but to obtain bounds further analytic techniques are required.

A. Is $\sigma_{\text{disc}}(H)$ infinite or finite?

The min–max principle is useful for establishing the existence of eigenvalues, in particular in showing that $H_0 + V$ has an infinite discrete spectrum in certain cases. We shall first prove a result in the two-body case. Intuitively, if there are an infinite number of bound states, those with small binding energy should be spatially spread out and so should be more sensitive to the large x behavior of $V(x)$ than the small x behavior. We thus expect in the two-body case that the question of whether or not $H_0 + V$ has an infinity of bound states to depend on the large x behavior of V. We shall

see that the borderline behavior is $|x|^{-2}$. The proof will depend on three things besides the min–max principle: (1) the "uncertainty principle lemma" of Section X.2, i.e., $-\Delta - \frac{1}{4}r^{-2} \geq 0$; (2) that $\sigma_{ess}(-\Delta + V) = [0, \infty)$ when $V \in R + (L^\infty)_\varepsilon$ where R is the Rollnik class: we shall prove this in the next section; (3) that $-\Delta + V$ has only finitely many bound states when $V \in R$; we shall prove this in Part C below.

Theorem XIII.6 Consider the operator $-\Delta + V$ on $L^2(\mathbb{R}^3)$.

(a) Suppose that $V \in R + (L^\infty)_\varepsilon$ and that V satisfies

$$V(x) \leq -ar^{-2+\varepsilon} \qquad \text{if} \quad r \equiv |x| > R_0$$

for some R_0 and some $a > 0$, $\varepsilon > 0$. Then $\sigma_{disc}(-\Delta + V)$ is infinite.

(b) Suppose that $V \in R + (L^\infty)_\varepsilon$ and that V satisfies

$$V(x) \geq -\tfrac{1}{4}br^{-2} \qquad \text{if} \quad r > R_0$$

for some R_0 and some $b < 1$. Then $\sigma_{disc}(-\Delta + V)$ is finite.

Proof (a) Since $\sigma_{ess}(-\Delta + V) = [0, \infty)$, it is sufficient to show $\mu_n < 0$ for each n. Pick a nonnegative C^∞ function ψ with support in $\{x \mid 1 < |x| < 2\}$ and $\|\psi\| = 1$. Let $\psi_R(x) = R^{-3/2}\psi(xR^{-1})$ so $\|\psi_R\| = 1$ and $\operatorname{supp} \psi_R \subset \{x \mid R < r < 2R\}$. If $R > R_0$, we conclude that

$$\begin{aligned}(\psi_R, H\psi_R) &= (\psi_R, -\Delta\psi_R) + (\psi_R, V\psi_R)\\ &\leq (\psi_R, -\Delta\psi_R) - a(\psi_R, r^{-2+\varepsilon}\psi_R)\\ &= R^{-2}(\psi, -\Delta\psi) - aR^{-2+\varepsilon}(\psi, r^{-2+\varepsilon}\psi)\end{aligned}$$

Since $\varepsilon > 0$, this last expression is negative for large R. Thus we can find Q so that $(\psi_R, H\psi_R) < 0$ if $R > Q$. Now let $\varphi_n = \psi_{2^nQ}$, $n = 1, 2, \ldots$. The φ_n are orthonormal and $(\varphi_n, H\varphi_m) = 0$ if $n \neq m$ since φ_n and φ_m have disjoint supports if $n \neq m$. Thus, given N, and taking $V_N = \operatorname{span}\{\varphi_1, \ldots, \varphi_N\}$, we see that $P_N H P_N \restriction V_N$ has eigenvalues $\{(\varphi_n, H\varphi_n)\}_{n=1}^N$. By the Rayleigh–Ritz principle

$$\mu_N(H) \leq \sup_{1 \leq m \leq N} \{(\varphi_m, H\varphi_m)\} < 0$$

Since N is arbitrary and $\sigma_{ess} = [0, \infty)$, $-\Delta + V$ has an infinity of eigenvalues.

(b) Let $W = V + \frac{1}{4}br^{-2}$. Then as forms on $Q(H_0)$,

$$\begin{aligned}-\Delta + V &= -(1-b)\Delta + W + b(-\Delta - \tfrac{1}{4}r^{-2})\\ &\geq -(1-b)\Delta + W\\ &\geq -(1-b)\Delta + \tilde{W}\end{aligned}$$

where $\tilde{W} = \min(W, 0)$. Thus by the min–max principle

$$\mu_n(-\Delta + V) \geq \mu_n(-(1-b)\Delta + \tilde{W}) = (1-b)\mu_n(-\Delta + (1-b)^{-1}\tilde{W})$$

By hypothesis, $\tilde{W}$ has compact support and lies in $R + (L^\infty)_\varepsilon$. A simple exercise (Problem 70 of Chapter XI) shows that if a potential in $R + (L^\infty)_\varepsilon$ has compact support, it is in R. Thus $-\Delta + (1-b)^{-1}\tilde{W}$ has only finitely many bound states, so $\mu_n(-\Delta + (1-b)^{-1}\tilde{W}) = 0$ for $n \geq N_0$ for some N_0. Thus

$$0 \geq \mu_n(-\Delta + V) \geq (1-b)\mu_n(-\Delta + (1-b)^{-1}\tilde{W}) = 0$$

if $n \geq N_0$. Therefore, $-\Delta + V$ has at most N_0 eigenvalues in $(-\infty, 0)$. ∎

Looking back at the proof, we can see why r^{-2} is the critical borderline behavior. $-\Delta$ scales as a homogeneous function of degree -2 under the scaling $\psi \to \psi_R$. Thus, if V scales at large distances with degree $-2+\varepsilon$, it wins out; and if it scales with degree $-2-\varepsilon$, the kinetic energy wins out and spread-out states cannot have negative energy.

For N-body systems, the situation is more complicated and is not merely dependent on the long-range behavior of V. For example, there is a three-body system with two-body potentials, $V = V_{01}(r_1) + V_{02}(r_2) + V_{12}(r_1 - r_2)$, so that the number of bound states $N(\lambda)$ of $H_\lambda = -\Delta_1 - \Delta_2 + \lambda V$ has the following behavior: For $\lambda = 0$, $N(\lambda) = 0$; as λ is increased from 0, $N(\lambda)$ increases one by one until suddenly at $\lambda = \lambda_1$, $N(\lambda) = \infty$. As λ is increased further, a new critical value λ_2 is reached; $N(\lambda) = \infty$ if $\lambda_1 \leq \lambda \leq \lambda_2$. As λ is further increased, new critical values λ_3, $\lambda_4, \ldots$ enter so that $N(\lambda) = \infty$ if $\lambda \in [\lambda_1, \lambda_2] \cup [\lambda_3, \lambda_4] \cup [\lambda_5, \lambda_6] \cup \cdots$ and $N(\lambda) < \infty$ if $\lambda \in [0, \lambda_1) \cup (\lambda_2, \lambda_3) \cup (\lambda_4, \lambda_5) \cup \cdots$. A reference for this example appears in the Notes.

The complicating feature of N-body systems is that their essential spectrum is $[\Sigma, \infty)$ where $\Sigma < 0$ is possible (see Section 5). Thus, in the example mentioned above $\mu_n(H_{\lambda_2}) < \Sigma_{\lambda_2}$ for all n. As λ is increased past λ_2, $\mu_n(H_\lambda)$ decreases below $\mu_n(H_{\lambda_2})$; but Σ_λ decreases also and can overtake $\mu_n(H_\lambda)$ so that for $\lambda > \lambda_2$, $\mu_n(H_\lambda) = \Sigma_\lambda$ for n large.

Let us consider the Hamiltonian of the helium atom. Heuristically, states in the essential spectrum should not be bound and thus should involve clusterings of particles far from one another. For example, electron one might be bound while two goes to ∞. Such states will have energy beginning at -1, the ground state energy of $-\Delta_1 - 2|r_1|^{-1}$. Considering the other possibilities, one sees that $\sigma_{\text{ess}}(H) = [-1, \infty)$ is to be expected on physical grounds. In fact, we shall prove this in Section 5. Knowing this, we can now show how the min–max principle can be used in the many-body case:

Proposition (Kato)

$$H = -\Delta_1 - 2|r_1|^{-1} - \Delta_2 - 2|r_2|^{-1} + |r_1 - r_2|^{-1}$$

has an infinite discrete spectrum.

Proof We need only show that $\mu_n(H) < -1$ for all n since $\sigma_{\text{ess}}(H) = [-1, \infty)$. By the Rayleigh–Ritz method, we need only find, for any n, an n-dimensional space V_n with $\sup(\psi, H\psi) < -\|\psi\|^2$ for all $\psi \in V_n$. Intuitively, we should find V_n by putting electron one in its ground state and putting electron two in a suitable state. Let $\psi_1(r_1)$ be the normalized ground state of $-\Delta_1 - 2|r_1|^{-1}$, i.e., $(-\Delta_1 - 2|r_1|^{-1})\psi_1 = -\psi_1$, and let $\varphi_n(r_2)$ be the normalized nth eigenfunction of $-\Delta_2 - |r_2|^{-1}$, i.e. $(-\Delta_2 - |r_2|^{-1})\varphi_n = E_n\varphi_n$ where $E_1, E_2, \ldots = -\frac{1}{4}, -\frac{1}{16}, -\frac{1}{16}, \ldots$, where $-(4n^2)^{-1}$ is repeated n^2 times. Now let $\psi = \sum_{i=1}^{n} \alpha_i \psi_1(r_1)\varphi_i(r_2)$ with $\sum_{i=1}^{n} |\alpha_i|^2 = 1$. Then $(\psi, H\psi) = t_1 + t_2 + t_3$ where

$$t_1 = (\psi, (-\Delta_1 - 2|r_1|^{-1})\psi) = (\psi, -\psi) = -1$$

$$t_2 = (\psi, (-\Delta_2 - |r_2|^{-1})\psi) = \sum_{i=1}^{n} |\alpha_i|^2 E_i \leq E_n$$

$$t_3 = (\psi, |r_1 - r_2|^{-1} - |r_2|^{-1})\psi) \leq 0$$

The last inequality $t_3 \leq 0$ follows from the fact that $\psi_1(r_1)$ is spherically symmetric so

$$\int |r_1 - r_2|^{-1} |\psi_1(r_1)|^2 \, dr_1 = \int \min\{|r_1|^{-1}, |r_2|^{-1}\} |\psi_1(r_1)|^2 \, dr_1$$

$$\leq |r_2|^{-1}$$

Thus, letting $V_n = \text{span}\{\psi_1\varphi_1, \ldots, \psi_1\varphi_n\}$, we see that

$$(\psi, H\psi) \leq -1 + E_n$$

if $\psi \in V_n$. Thus $\mu_n(H) \leq -1 + E_n < -1$. This shows that $\sigma_{\text{disc}}(H)$ is an infinite set. ∎

The above arguments have been extended in various directions. Typical of the results is:

Theorem XIII.7 (Zhislin) Let H be an "atomic" Hamiltonian of the form

$$H = \sum_{i=1}^{n} \left(-\frac{\Delta_i}{2\mu_i} - \frac{n}{|r_i|} \right) + \sum_{i<j} \left(\frac{\nabla_i \cdot \nabla_j}{M} + \frac{1}{|r_i - r_j|} \right)$$

as an operator on $L^2(\mathbb{R}^{3n})$ where M, $\{\mu_i\}_{i=1}^n$ are arbitrary positive numbers. Then $\sigma_{\text{disc}}(H)$ is infinite.

H is the Hamiltonian of a system consisting of a nucleus of mass M and n electrons of masses $\mu_1, \ldots, \mu_n$ after the center of mass motion is removed.

B. Bounds on $N(V)$ in the central case

Recall that a **central potential** is a real-valued function that is a function of $r = |x|$ alone. In that case, if E is an eigenvalue of $H = -\Delta + V$, then $\{\psi \mid H\psi = E\psi\}$ is a rotationally invariant subspace of $L^2(\mathbb{R}^3)$ and so is spanned by vectors of the form $\psi(x) = r^{-1}f(r)Y_{\ell m}(\theta, \varphi)$ where $Y_{\ell m}$ are the spherical harmonics and $\int_0^\infty |f(r)|^2\, dr < \infty$. ℓ is called the **angular momentum** of ψ. If $\psi \in D(H_0)$, it is bounded and continuous, so $f(r)$ is continuous and $f(0) = 0$. Moreover, f obeys the differential equation

$$\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r)\right) f(r) = Ef(r) \tag{4}$$

(4) holds in the sense of a differential operator on $L^2(0, \infty)$ with boundary condition $f(0) = 0$ rather than in the sense of classical differential equations. To avoid troubles with this fact, we shall suppose that V is C^∞ with compact support. The elliptic regularity theorem then implies that solutions of (4) are C^∞. We shall later see how to remove the C_0^∞ assumption when we pass to the bounds. Alternatively, we could use the Jost function methods of Section XI.8 and allow fairly general V's throughout.

For any integral ℓ and $E \leq 0$, let $u_\ell(r; E)$ be the solution of (4) obeying $u_\ell(0; E) = 0$ and $\lim_{r \downarrow 0} r^{-\ell-1}u_\ell(r; E) = 1$. The existence and uniqueness of such solutions when $V \in C_0^\infty$ is fairly easy (see Section XI.8). We are interested in the number of $E < 0$ for which $u_\ell(r; E)$ is square integrable. This is precisely $n_\ell(V)$, the "number" of discrete bound states of $-\Delta + V$ with angular momentum ℓ, in the sense that for fixed ℓ *and* m it is the number of discrete bound states of the form $r^{-1}f(r)Y_{\ell m}(\theta, \varphi)$. Since m can equal $-\ell$, $-\ell + 1, \ldots, \ell$ there are really $(2\ell + 1)n_\ell(V)$ discrete eigenfunctions of angular momentum ℓ, so $N(V) = \sum (2\ell + 1)n_\ell(V)$. There is a classical theorem about $n_\ell(V)$:

Theorem XIII.8 Suppose that $V \in C_0^\infty(0, \infty)$ and let $N_\ell(E; V)$ be the number of zeros of $u_\ell(r; E)$ different from $r = 0$. Then:

(a) If $E < 0$, then $N_\ell(E; V) < \infty$.

(b) $N_\ell(E; V)$ is a monotone increasing function of E and a monotone decreasing function of ℓ.

(c) If $E_0 \leq 0$, $N_\ell(E_0; V)$ is identical to the number of square integrable solutions of (4) with $E < E_0$. In particular, $n_\ell(V) = N_\ell(0; V)$ and $\dim P_{(-\infty, E)} = \sum_{\ell=0}^{\infty} (2\ell + 1) N_\ell(E; V)$ for $E \leq 0$ where $\{P_\Omega\}$ are the spectral projections for $-\Delta + V(|x|)$.

We shall prove this theorem in a sequence of lemmas. While the classical proof uses notions from the theory of differential equations, we are able to avoid most of this machinery by appealing to the min–max principle several times. Before turning to the proof, let us explain why there should be a connection between N_ℓ and n_ℓ. Suppose E is so negative that $E - V$ is everywhere negative. By the differential equation, u and u'' have the same sign. So, if u and u' start out positive, they remain positive. Thus $N_\ell(E; V) = 0$ if E is very negative. We shall see that as E decreases from $E = 0$, the zeros of $u_\ell(r; E)$ move to larger r. They disappear by moving out to $r = \infty$. Since $N_\ell(E; V) = 0$ for E very negative, $N_\ell(0; V)$ is the number of zeros that have moved out to infinity. The point is that those energies at which zeros have just moved out to infinity are intuitively precisely those energies for which $\lim_{r\to\infty} u_\ell(r; E) = 0$. Since V has compact support, $u_\ell(r; E) \sim a \exp(-\sqrt{-E}\, r) + b \exp(+\sqrt{-E}\, r)$ for r large. If

$$\lim_{r\to\infty} u_\ell(r; E) = 0,$$

$u_\ell(r; E) \sim a \exp(-\sqrt{-E}\, r)$ for r large, so u_ℓ is square integrable. So the number of eigenvalues should be the number of zeros.

Lemma 1 Let $E_0 \leq 0$. If $N_\ell(E_0; V) \geq m_0$, then (4) has at least m_0 square integrable solutions with $E < E_0$. In particular, since $\sigma_{\text{ess}}(-\Delta + V) = [0, \infty)$, $N_\ell(E_0; V) < \infty$ if $E_0 < 0$.

Proof Let

$$H_\ell = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r)$$

as an operator on $L^2(0, \infty)$. It is essentially self-adjoint with domain $\{u \,|\, u \in C_0^\infty[0, \infty); u(0) = 0\}$ if $\ell = 0$ and on $\{u \,|\, u \in C_0^\infty(0, \infty)\}$ if $\ell \neq 0$ (Problem 16). We shall first show if $N_\ell(E_0; V) \geq m_0$, then $\mu_{m_0}(H_\ell) \leq E_0$. For let $r_0 = 0 < r_1 < r_2 < \cdots < r_{m_0} < \infty$ be zeros of $u_\ell(r; E_0)$. Define ψ_i by

$$\psi_i(r) = \begin{cases} u_\ell(r; E_0), & r_{i-1} \leq r \leq r_i \\ 0, & \text{otherwise} \end{cases}$$

Then the ψ_i are continuous and piecewise C^1. While $\psi_i \notin D(-d^2/dr^2)$, it is in $Q(-d^2/dr^2)$ and so in $Q(H_\ell)$ (see Problem 17). Moreover

$$\left(\sum_{i=1}^{m_0} a_i\psi_i\,,\, H_\ell \sum_{i=1}^{m_0} a_i\psi_i\right) = \left(\frac{d}{dr}\left(\sum_{i=1}^{m_0} a_i\psi_i\right),\, \frac{d}{dr}\left(\sum_{i=1}^{m_0} a_i\psi_i\right)\right)$$

$$+ \left(\sum_{i=1}^{m_0} a_i\psi_i\,,\, \left(\frac{\ell(\ell+1)}{r^2} + V\right)\sum_{i=1}^{m_0} a_i\psi_i\right)$$

$$= \sum_{i=1}^{m_0} |a_i|^2 \int_{r_{i-1}}^{r_i} \left[|\psi_i'|^2 + \left(\frac{\ell(\ell+1)}{r^2} + V\right)|\psi_i|^2\right] dr$$

$$= \sum_{i=1}^{m_0} |a_i|^2 \int_{r_{i-1}}^{r_i} \bar{\psi}_i\left[-\psi_i'' + \left(\frac{\ell(\ell+1)}{r^2} + V\right)\psi_i\right] dr$$

$$= E_0\left(\sum_{i=1}^{m_0} a_i\psi_i\,,\, \sum_{i=1}^{m_0} a_i\psi_i\right)$$

Thus we have an m_0-dimensional subspace of $Q(H_\ell)$ on which the expectation value of H_ℓ is less than or equal to E_0, so $\mu_{m_0}(H_\ell) \leq E_0$, by Theorem XIII.2.

Next, we note that if $E_n \to E_\infty$, then $u_\ell(r; E_n)$ converges to $u_\ell(r; E_\infty)$ uniformly on compact subsets of $[0, \infty)$. This is because of the continuity of solutions of ordinary differential equations in their coefficients. Thus $u_\ell(r; E_0 - 1/n)$ converges uniformly on compacts to $u_\ell(r; E_0)$. It follows that if $u_\ell(r; E_0)$ has at least m_0 zeros, then for some n, $u_\ell(r; E_0 - 1/n)$ has at least m_0 zeros so $\mu_{m_0}(H_\ell) \leq E_0 - 1/n < E_0$. Since $\sigma_{\text{ess}}(H_\ell) \subset \sigma_{\text{ess}}(-\Delta + V) = [0, \infty)$, the lemma follows from the min–max principle. ∎

Lemma 2 (Sturm oscillation theorem) $N_\ell(E; V)$ is a monotone increasing function of E. If $E_0 < 0$ is an eigenvalue of H_ℓ, then $N_\ell(E; V) \geq N_\ell(E_0; V) + 1$ when $E > E_0$.

Proof Let $V_\ell = \ell(\ell+1)r^{-2} + V$ and let $r_0 = 0 < r_1 < \cdots < r_n < \infty$ be the zeros of $u_\ell(r; E_0)$. Let $E > E_0$. We shall show that $u_\ell(r, E)$ has at least one zero in each of the intervals $(0, r_1), (r_1, r_2), \ldots, (r_{n-1}, r_n)$ and when E_0 is an eigenvalue, also in the interval (r_n, ∞). For suppose $u_\ell(r; E)$ has no zero in (r_i, r_{i+1}). By replacing u_ℓ with $-u_\ell$ if necessary, we can suppose that both $u_\ell(r; E)$ and $u_\ell(r; E_0)$ are nonnegative in (r_i, r_{i+1}). In particular, $u_\ell'(r_i; E_0) \geq 0$ and $u_\ell'(r_{i+1}; E_0) \leq 0$. Let us compute

$$I = \int_{r_i}^{r_{i+1}} [u_\ell'(r; E_0)u_\ell(r; E) - u_\ell(r; E_0)u_\ell'(r; E)]'\, dr$$

On one hand

$$I = [u'_\ell(r; E_0)u_\ell(r; E) - u_\ell(r; E_0)u'_\ell(r; E)]\Big|_{r_i}^{r_{i+1}}$$

$$= u'_\ell(r_{i+1}; E_0)u_\ell(r_{i+1}; E) - u'_\ell(r_i; E_0)u_\ell(r_i; E)$$

$$\leq 0$$

On the other hand

$$I = \int_{r_i}^{r_{i+1}} [u''_\ell(r; E_0)u_\ell(r; E) - u_\ell(r; E_0)u''_\ell(r; E)]\, dr$$

$$= \int_{r_i}^{r_{i+1}} u_\ell(r; E_0)u_\ell(r; E)[(V_\ell - E_0) - (V_\ell - E)]\, dr$$

$$= (E - E_0)\int_{r_i}^{r_{i+1}} u_\ell(r; E_0)u_\ell(r; E)\, dr > 0$$

This contradiction shows that $u_\ell(r, E)$ must have a zero in (r_i, r_{i+1}). Now suppose E_0 is an eigenvalue and $\ell = 0$. Since V has compact support, $u_0(r, E_0) = a \exp(-\sqrt{-E_0}\, r)$ for r large and $|u_0(r; E)| + |u'_0(r; E)| \leq b \exp(+\sqrt{-E}\, r)$ for r large. As a result, the integrals I and the other integrals we wrote down above converge if we replace r_{i+1} with ∞ and r_i with r_n. Thus $u_0(r; E)$ has a zero in (r_n, ∞) by the same reasoning. A similar argument works for general ℓ if we replace the exponential by suitable Bessel functions. We conclude that the lemma is valid. ∎

Lemma 3 $N_\ell(\mu_n(H_\ell); V) = n - 1$ if $\mu_n(H_\ell) < 0$.

Proof If $N_\ell(\mu_n(H_\ell); V) > n - 1$, then, by Lemma 1, there are at least n eigenvalues in $(-\infty, \mu_n)$, so we see that $N_\ell(\mu_n(H_\ell)) \leq n - 1$ by the min–max principle. On the other hand, we shall prove that $N_\ell(\mu_n(H_\ell)) \geq n - 1$ by induction. Certainly $N_\ell(\mu_1(H_\ell)) \geq 0$. Suppose $\mu_n < 0$ and $N_\ell(\mu_{n-1}(H_\ell)) \geq n - 2$. Since $\mu_{n-1} \leq \mu_n < 0$, μ_{n-1} is an eigenvalue and μ_n is an eigenvalue, so $\mu_n > \mu_{n-1}$ since (4) can have at most one solution with $f(0) = 0$. Thus, by Lemma 2,

$$N_\ell(\mu_n(H_\ell)) \geq N_\ell(\mu_{n-1}(H_\ell)) + 1 = n - 1 \quad ∎$$

We are now ready for

Proof of Theorem XIII.8 We have already proven (a) and that $N_\ell(E; V)$ is monotone in E. On one hand, by Lemma 1, the number of bound states with

energy less than E is not smaller than $N_\ell(E; V)$. On the other hand, suppose it is larger than $N_\ell(E; V)$. This is impossible if $E = 0$ and $N_\ell = \infty$, so suppose $N_\ell(E; V) = n < \infty$. We are supposing that there are $n + 1$ eigenvalues below E so $\mu_{n+1}(H_\ell) < E$. But $N_\ell(\mu_{n+1}(H_\ell)) = n$ and μ_{n+1} is an eigenvalue; so by Lemma 2, $N_\ell(E; V) \geq n + 1$. This contradiction shows that $N_\ell(E; V)$ is the number of eigenvalues of H_ℓ in $(-\infty, E)$. Since $H_{\ell+1} \geq H_\ell$, we conclude $N_\ell(E; V) \geq N_{\ell+1}(E; V)$. ∎

We can use Theorem XIII.8 to prove a variety of bounds on $n_\ell(V)$ and on $\ell_{\max}(V) = \max\{\ell \mid n_\ell(V) > 0\}$, the largest angular momentum that has bound states:

Theorem XIII.9 Let V be a central potential with $V \in R + L^\infty(\mathbb{R}^3)_\varepsilon$. Then:

(a) (Bargmann's bound)

$$n_\ell(V) \leq (2\ell + 1)^{-1} \int_0^\infty r\,|V(r)|\,dr$$

(b) (Calogero's bound) Suppose V is monotone increasing and negative. Then

$$n_\ell(V) \leq \frac{2}{\pi} \int_0^\infty |V(r)|^{1/2}\,dr$$

(c) (the GGMT bound) For any $p \geq 1$,

$$n_\ell(V) \leq c_p(2\ell + 1)^{-(2p-1)} \int_0^\infty r^{2p-1}\,|V(r)|^p\,dr$$

where $c_p = (p-1)^{p-1}\Gamma(2p)/p^p\Gamma(p)^2$ and Γ is the Euler gamma function.

(d) If $\int_0^\infty |V(r)|^{1/2}\,dr < \infty$ and if $V(r) < 0$ on some open set, then for each ℓ, there exist Λ, a, and b with $0 < a < b < \infty$ so that if $\lambda > \Lambda$,

$$a\lambda^{1/2} \leq n_\ell(\lambda V) \leq b\lambda^{1/2}$$

(e) If $\int_0^\infty r\,|V(r)|\,dr < \infty$ and $V(r) < 0$ on an open set, then there are c, d, and Λ with $0 < c < d < \infty$ so that if $\lambda > \Lambda$,

$$c\lambda^{1/2} \leq \ell_{\max}(\lambda V) \leq d\lambda^{1/2}$$

Proof We shall prove only Bargmann's bound in case $\ell = 0$ (see Problem 19 and the references in the Notes for other parts of the proof). We first remark that it is enough to prove the bound when $V \leq 0$. For let V be

arbitrary and let $V_- = \min\{V, 0\}$. Then by the min–max principle, $n_\ell(V_-) \geq n_\ell(V)$ since $-\Delta + V_- \leq -\Delta + V$. Thus, if we know $n_0(V_-) \leq \int_0^\infty r\,|V_-(r)|\,dr$, we can conclude

$$n_0(V) \leq n_0(V_-) \leq \int_0^\infty r\,|V_-(r)|\,dr \leq \int_0^\infty r\,|V(r)|\,dr \tag{5}$$

Next we remark that we need prove only the theorem for the case where $V \in C_0^\infty$ and is nonpositive, for an arbitrary $V \in R + (L^\infty)_\varepsilon$ with $V \leq 0$ and $\int_0^\infty r\,|V(r)|\,dr < \infty$ can be approximated by nonpositive $V_n \in C_0^\infty$ in such a way that $\int_0^\infty r\,|V_n(r)|\,dr| \uparrow \int_0^\infty r\,|V(r)|\,dr$ and $V_n - V \to 0$ in $R + L^\infty$. Since $V_n - V \to 0$ in $R + L^\infty$, $-\Delta + V_n \to -\Delta + V$ in norm resolvent sense. Thus $P^{(n)}_{(-\infty, E)} \to P_{(-\infty, E)}$ for any $E < 0$ not an eigenvalue of $-\Delta + V$. Letting $P^{(\ell)}$ be the projection onto states of angular momentum ℓ, we conclude that

$$\lim_{E \uparrow 0} \operatorname{Tr}[P^{(n)}_{(-\infty, E)} P^{(\ell)}] = (2\ell + 1) n_\ell(V_n)$$

where the left-hand side converges monotonically and

$$\lim_{E \uparrow 0} \operatorname{Tr}[P_{(-\infty, E)} P^{(\ell)}] = (2\ell + 1) n_\ell(V_n)$$

If we know $n_0(V_n) \leq \int_0^\infty r\,|V_n(r)|\,dr$, we can conclude that

$$\begin{aligned} n_0(V) = \lim_{E \uparrow 0} \operatorname{Tr}[P_{(-\infty, E)} P^{(0)}] &\leq \sup_{n,\, E<0} \operatorname{Tr}[P^{(n)}_{(-\infty, E)} P^{(0)}] \\ &\leq \sup_n n_0(V_n) \leq \sup_n \int_0^\infty r\,|V_n(r)|\,dr \\ &= \int_0^\infty r\,|V(r)|\,dr \end{aligned}$$

It is the above argument that allows us to deal only with $V \in C_0^\infty$ in Theorem XIII.8. Henceforth we suppose that $V \in C_0^\infty$ and $V \leq 0$.

Let u be the solution of $-u'' + Vu = 0$ with $u(0) = 0$. Let us define

$$a(r) = \frac{u(r)}{u'(r)} - r$$

where $u'(r) \neq 0$. Then $u(r) = (a(r) + r)u'(r)$ so

$$\begin{aligned} u'(r) &= (a'(r) + 1)u'(r) + (a(r) + r)u''(r) \\ &= u'(r) + a'(r)u'(r) + V(r)(a(r) + r)u(r) \\ &= u'(r) + a'(r)u'(r) + V(r)(a(r) + r)^2 u'(r) \end{aligned}$$

Thus, when $u'(r) \neq 0$

$$a'(r) = -V(r)(a(r) + r)^2 \tag{6}$$

which is called the **Riccati equation**. The passage from the second-order linear equation $-u'' + Vu = 0$ to a first-order nonlinear differential equation like (6) is the first important element of the proof. The value of such equations is that they become first-order differential inequalities by dropping positive terms and can then be integrated to yield inequalities on the number of zeros of $u(r)$.

Since $V \leq 0$, a is monotone increasing by (6) and a goes to infinity at each zero of $u'(r)$. Since a is monotone, the number of poles of $a(r)$ is precisely the number of zeros of $a(r) + r$ (see Figure XIII.1). By Theorem XIII.8, the number of zeros of $u(r)$, which is the number of zeros of $a(r) + r$, is precisely $n_0(V)$. We have used the fact that u obeys a second-order equation so u and u' cannot both vanish simultaneously at a point $r \neq 0$.

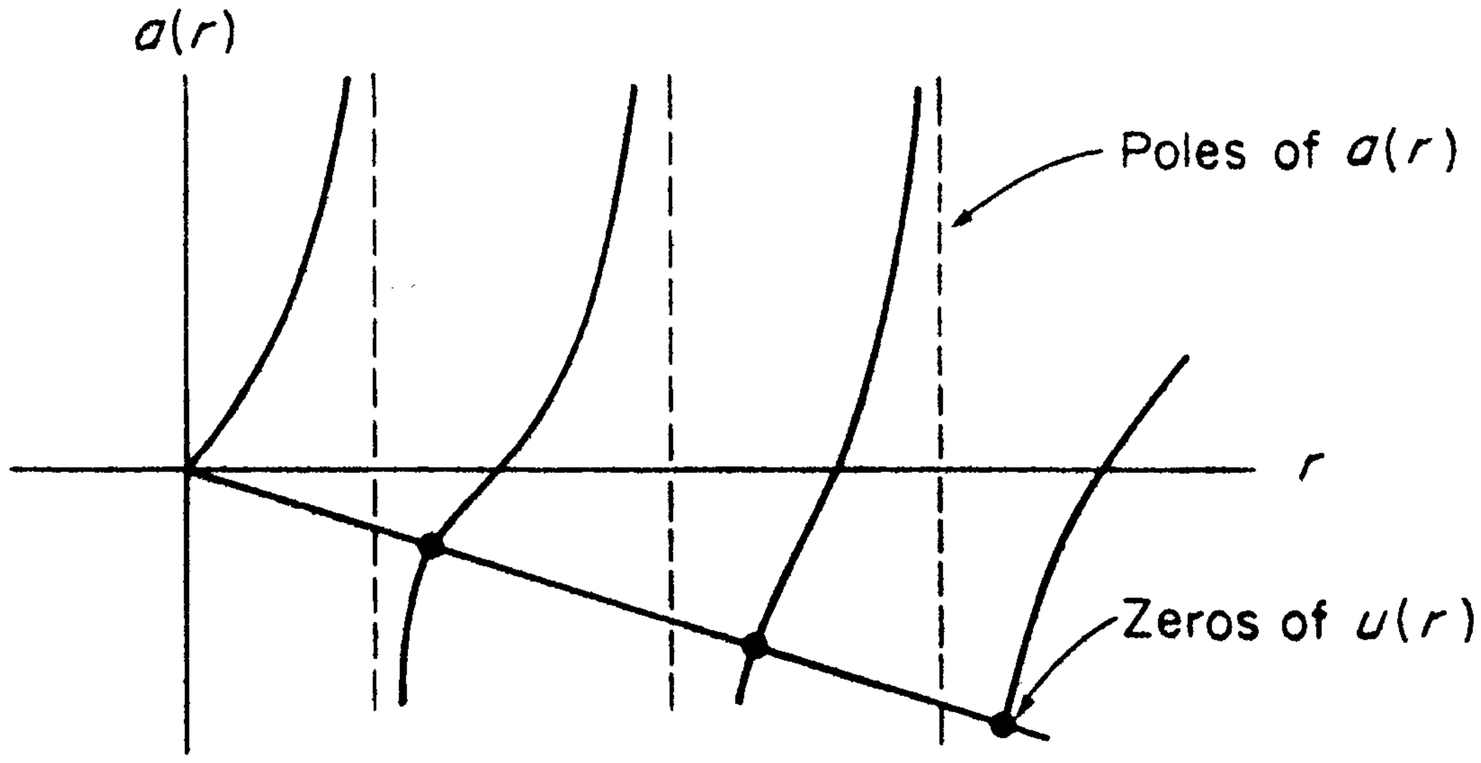


FIGURE XIII.1 The Ricati function $a(r)$.

The trick of proving both Bargmann's bound and Calogero's bound is to introduce an auxiliary function of a, write down its differential equation, and integrate a related differential inequality (see Problem 18 for Calogero's bound). Let $b(r) = a(r)/r$. Then (6) implies

$$b'(r) = -rV(r)(b(r) + 1)^2 - r^{-1}b(r)$$

Moreover, $b(0) = 0$ since $a(0) = \lim_{r\to 0} (u(r)/u'(r) - r) = 0$ and so $\lim_{r\to 0} b(r) = \lim_{r\to 0} a'(r) = 0$ by (6). Finally the poles of $b(r)$ are precisely the poles of $a(r)$, so the number of poles of b is $n_0(V)$. Suppose that b has zeros $z_1 = 0 < z_2 < \cdots < z_n$ and poles $p_1 < p_2 < \cdots < p_n$ with $z_i < p_i < z_{i+1}$. Then in each interval (z_i, p_i), $b(r) > 0$ so

$$b'(r) \leq -rV(r)(b(r) + 1)^2$$

or

$$-[(1 + b(r))^{-1}]' \leq -rV(r) = r\,|V(r)|$$

since $V \leq 0$. Integrating from z_i to p_i,

$$1 = \int_{z_i}^{p_i} -\frac{d}{dr}\left(\frac{1}{1 + b(r)}\right) dr \leq \int_{z_i}^{p_i} r\,|V(r)|\; dr$$

Summing over i,

$$n_0(V) \leq \sum_{i=1}^{n} \int_{z_i}^{p_i} r\,|V(r)|\; dr \leq \int_0^{\infty} r\,|V(r)|\; dr$$

which proves the bound. ∎

There are several remarks to be made about the bounds in Theorem XIII.9. First, by the argument leading to (5), the bounds

$$n_\ell(V) \leq (2\ell + 1)^{-1} \int_0^{\infty} r\,|V_-(r)|\; dr$$

and

$$n_\ell(V) \leq \frac{2}{\pi} \int_0^{\infty} |V_-(r)|^{1/2}\; dr$$

hold. Secondly, Bargmann's bound tells us that if $\int_0^\infty r\,|V(r)|\; dr < \infty$, then $n_\ell(V) = 0$ for ℓ large since $n_\ell(V) = 0$ if it is less than 1. Explicitly, Bargmann's bound implies

$$\ell_{\max}(V) \leq \tfrac{1}{2}\left[\int_0^{\infty} r\,|V(r)|\; dr - 1\right] \tag{7}$$

Next we note that Bargmann's bound, Calogero's bound, and (7) are "best possible" in the sense that there exist potentials with $n_\ell(V)$ (or $\ell_{\max}(V)$) any preassigned integer and with the integral on the right-hand side arbitrarily close to $n_\ell(V)$ (or $\ell_{\max}(V)$). Thus, the constants $(2\ell + 1)^{-1}$, $2/\pi$, and $1/2$ cannot be replaced with smaller constants. On the other hand, Bargmann's bound and (7) are very poor for strong potentials in the sense that as $\lambda \to \infty$, the bounds grow like λ while $n_\ell(\lambda V)$ and $\ell_{\max}(\lambda V)$ grow like $\lambda^{1/2}$. Finally, we remark that (d) and (e) can be improved for restricted classes of potentials:

$$\lim_{\lambda \to \infty} \frac{n_\ell(\lambda V)}{\lambda^{1/2}} = \frac{1}{\pi} \int_0^{\infty} |V_-(r)|^{1/2}\; dr \tag{8}$$

for any ℓ,

$$\lim_{\lambda \to \infty} \frac{\ell_{\max}(\lambda V)}{\lambda^{1/2}} = -\min_r \{r^2 V(r)\}$$

and

$$\lim_{\lambda \to \infty} \frac{N(\lambda V)}{\lambda^{3/2}} = \frac{1}{6\pi^2} \int |V_-(r)|^{3/2} \, d^3r \tag{9}$$

We shall prove (8) and (9) under very general circumstances in Section 15.

C. Bounds on $N(V)$ in the general two-body case

We now turn to proving bounds on $N(V)$, the total number of bound states, without supposing V is central. We first note two useful facts:

Lemma Let H_0 be self-adjoint and positive. Let V be a form-bounded perturbation of H_0 with relative bound zero. Let $H_0 + \lambda V$ be defined as the operator arising from the sum of forms ($\lambda \in \mathbb{R}$). Suppose that $[0, \infty) \subset \sigma(H_0 + \lambda V)$ for all $\lambda \in \mathbb{R}$. Then:

(a) $\mu_n(H_0 + \lambda V)$ is continuous in λ for $\lambda \in \mathbb{R}$;
(b) $\mu_n(H_0 + \lambda V)$ is monotone decreasing in λ for $\lambda \in [0, \infty)$ and strictly monotone once μ_n is negative.

This lemma follows from an application of the min–max principle (Problem 25a). In the case of interest where $H_0 = -\Delta$, $V \in R + (L^\infty)_\varepsilon$, one can also use the perturbation theory of Chapter XII (Problem 25b). R is the Rollnik class defined in Volume II.

Theorem XIII.10 (the Birman–Schwinger bound) Let $V \in R$. Then

$$N(V) \leq \left(\frac{1}{4\pi}\right)^2 \int \frac{|V(x)|\,|V(y)|}{|x - y|^2} \, d^3x \, d^3y$$

In particular, $N(V) < \infty$.

Proof As in the proof of Theorem XIII.9, it is sufficient to prove the bound when V is in C_0^∞ and $V \leq 0$. Let $E < 0$ and let $N_E(V) = \dim(\text{Ran } P_{(-\infty, E)})$. For simplicity of notation, write $\mu_n(\lambda)$ for $\mu_n(-\Delta + \lambda V)$. Then

$$N_E(V) = \#\{n \,|\, \mu_n(1) < E\}$$

where $\#(A)$ is the cardinality of the set A. Since $\mu_n(\lambda)$ is monotone and continuous and $\mu_n(0) = 0$, $\mu_n(1) < E$ if and only if $\mu_n(\lambda) = E$ for some $0 < \lambda < 1$, and in that case $\mu_n(\lambda) = E$ for exactly one λ. Thus

$$N_E(V) = \#\{n \,|\, \mu_n(\lambda) = E \text{ for some } \lambda \in (0, 1)\}$$
$$\leq \sum_{\{\lambda | \mu_k(\lambda) = E;\, k = 1, \ldots, N_E(V)\}} \lambda^{-2} \leq \sum_{\{\lambda | \mu_k(\lambda) = E;\, k = 1, 2, \ldots\}} \lambda^{-2}$$

Next we note that $(H_0 + \lambda V - E)\psi = 0$ if and only if (Problem 26)

$$\lambda(|V|^{1/2}(H_0 - E)^{-1}|V|^{1/2})(|V|^{1/2}\psi) = (|V|^{1/2}\psi)$$

and this is true if and only if

$$\lambda \int \frac{|V(x)|^{1/2}\, e^{-\sqrt{-E}|x-y|}\, |V(y)|^{1/2}}{4\pi|x-y|} \varphi(y)\, dy = \varphi(x)$$

has a solution $\varphi \in L^2$ with $\varphi \neq 0$. Let K be the operator with integral kernel $|V(x)|^{1/2} \exp(-\sqrt{-E}|x-y|)|V(y)|^{1/2}/4\pi|x-y|$. Since $V \in R$, K is Hilbert–Schmidt and it is self-adjoint since the kernel is real and symmetric. As a result

$$\sum_{\{\mu | \mu \text{ is an eigenvalue of } K\}} \mu^2 = \operatorname{Tr}(K^*K)$$
$$= \left(\frac{1}{4\pi}\right)^2 \int e^{-2\sqrt{-E}|x-y|} \frac{|V(x)|\,|V(y)|}{|x-y|^2}\, dx\, dy$$

But a nonzero μ is an eigenvalue of K if and only if $\mu^{-1}K\varphi = \varphi$ has a solution, which by our above analysis is true if and only if $\mu_n(\lambda) = E$ with $\lambda = \mu^{-1}$. Thus

$$\sum_{\{\lambda | \mu_k(\lambda) = E\}} \lambda^{-2} = \sum_{\{\mu | \mu \text{ is an eigenvalue of } K\}} \mu^2$$

so

$$N_E(V) \leq \left(\frac{1}{4\pi}\right)^2 \int e^{-2\sqrt{-E}|x-y|} \frac{|V(x)|\,|V(y)|}{|x-y|^2}\, dx\, dy$$

Since $N(V) = \lim_{E \uparrow 0} N_E(V)$, the theorem is proven. ∎

As in the case of the central bounds, if one defines $V_- = \min(V, 0)$,

$$N(V) \leq \left(\frac{1}{4\pi}\right)^2 \int \frac{V_-(x)V_-(y)}{|x-y|^2}\, dx\, dy$$

We also note that the Birman–Schwinger bound can be extended to include zero energy bound states, i.e., one can prove (Problem 28):

$$\dim(\text{Ran } P_{(-\infty,0]}) \leq \left(\frac{1}{4\pi}\right)^2 \int \frac{|V(x)|\,|V(y)|}{|x-y|^2}\,dx\,dy$$

The method of proof used above can also be used to prove Bargmann's bound.

One consequence of the Birman–Schwinger bound is that, when $V \in C_0^\infty(\mathbb{R}^3)$, $N(\lambda V) = 0$ for sufficiently small λ. We shall see shortly that this is also true when $n > 3$. In fact, we shall prove in Section 7 that if $V \in L^{\frac{1}{2}n-\varepsilon}(\mathbb{R}^n) \cap L^{\frac{1}{2}n+\varepsilon}(\mathbb{R}^n)$, then $-\Delta + \lambda V$ and $-\Delta$ are unitarily equivalent for λ small. However, when $n = 1, 2$, the situation is different.

Theorem XIII.11 Let V be an everywhere nonpositive function in $C_0^\infty(\mathbb{R}^n)$, for $n = 1$ or 2, which is not identically zero. Then $-\Delta + \lambda V$ has a negative eigenvalue for all $\lambda > 0$.

Proof By the analysis in the proof of Theorem XIII.10, it suffices to prove that for any $\lambda > 0$, there is a κ for which $|V|^{1/2}(-\Delta + \kappa^2)^{-1}|V|^{1/2}$ has an eigenvalue larger than λ^{-1}. Since $|V|^{1/2}(-\Delta + \kappa^2)^{-1}|V|^{1/2}$ is a compact (in fact, Hilbert–Schmidt) operator that is positive and self-adjoint, it suffices to prove that

$$\lim_{\kappa^2 \to 0} \| |V|^{1/2}(-\Delta + \kappa^2)^{-1}|V|^{1/2} \| = \infty$$

To do this, we need only find $\eta \in L^2(\mathbb{R}^n)$ so that

$$\lim_{\kappa^2 \downarrow 0} (|V|^{1/2}\eta, (-\Delta + \kappa^2)^{-1}|V|^{1/2}\eta) = \infty$$

Choose any nonzero η in L^2 so that $\varphi(x) \equiv |V(x)|^{1/2}\eta(x) \geq 0$ and is not zero a.e. Then

$$(|V|^{1/2}\eta, (-\Delta + \kappa^2)^{-1}|V|^{1/2}\eta) = \int |\hat{\varphi}(p)|^2(p^2 + \kappa^2)^{-1}\,d^n p$$

Since $\hat{\varphi}(p) \neq 0$ for p near zero, and $n = 1$ or 2, this integral diverges as $\kappa^2 \to 0$. ∎

We shall discuss this phenomenon again in Section 17. There is more information in Problems 20–22. In particular, in the case just discussed it can be shown that $-\Delta + \lambda V$ has one negative eigenvalue for λ small.

We have already noted that the Bargmann bound has the wrong large coupling constant behavior in the sense that $n_\ell(\lambda V)$ grows like $c\lambda^{1/2}$ while

the bound grows like $c\lambda$. Similarly, in the Birman–Schwinger bound $N(V)$ grows like $c\lambda^{3/2}$, while the bound grows like $c\lambda^2$. This defect is remedied by the following result, which is especially pretty because of the connection with the classical phase-space picture discussed in Section 15.

Theorem XIII.12 (the Cwikel–Lieb–Rosenbljum bound) Let $n \geq 3$ and let $N(V)$ denote the number of bound states of $-\Delta + V$ on $L^2(\mathbb{R}^n)$. Then

$$N(V) \leq c_n \int |V_-(x)|^{n/2}\, d^n x \tag{10}$$

for suitable c_n.

Proof We consider the case $n = 3$ first and then describe the modifications necessary for $n \geq 4$. The first remark is that, as in the proof of the Birman–Schwinger bound, we can suppose that $V \leq 0$ and that $V \in C_0^\infty$. We thus let $W = -V \geq 0$.

For $E < 0$, let $N_E(V)$ denote the number of eigenvalues of $-\Delta - W = -\Delta + V$ below E. Let $H_0 = -\Delta$ and $E = -\kappa^2$. We claim that

$$N_E(V) \leq 2\,\mathrm{Tr}(W[(H_0 + \kappa^2)^{-1} - (H_0 + W + \kappa^2)^{-1}]) \tag{11}$$

For suppose that φ obeys $(H_0 - \lambda W)\varphi = E\varphi$. Then $\psi = W^{1/2}\varphi$ obeys

$$W^{1/2}(H_0 + \kappa^2)^{-1} W^{1/2}\psi = \lambda^{-1}\psi$$

$$W^{1/2}(H_0 + W + \kappa^2)^{-1} W^{1/2}\psi = (1 + \lambda)^{-1}\psi$$

and so letting

$$K = W^{1/2}[(H_0 + \kappa^2)^{-1} - (H_0 + W + \kappa^2)^{-1}]W^{1/2}$$

$$K\psi = [\lambda^{-1} - (1 + \lambda)^{-1}]\psi$$

As in the proof of the Birman–Schwinger bound, we see that $N_E(V)$, which is the number of λ's in $(0, 1]$ so that $(H_0 - \lambda W)\varphi = E\varphi$ has a solution (counting multiplicities), is bounded by the number of eigenvalues of K that are larger than $\frac{1}{2}$. Since K is a positive operator, this is bounded by $2\,\mathrm{Tr}(K)$ which is given by (11) on account of cyclicity of the trace.

Using (X.98), which relates resolvents to semigroups, we see that

$$N_E(V) \leq 2 \int_0^\infty \mathrm{Tr}(W[e^{-tH_0} - e^{-t(H_0+W)}])e^{Et}\, dt$$

where one can justify the interchange of the integral and Tr by using the bounds which we prove below. Since we shall also see that

$\mathrm{Tr}(W[e^{-tH_0} - e^{-t(H_0+W)}])$ is positive, and since $N(V) = \lim_{E \uparrow 0} N_E(V)$, we conclude that

$$N(V) \leq 2 \int_0^\infty \mathrm{Tr}(W[e^{-tH_0} - e^{-t(H_0+W)}])\, dt \tag{12}$$

by the monotone convergence theorem.

The key idea in the proof will be to realize $e^{-tH_0} - e^{-t(H_0+W)}$ as an integral operator using Wiener integrals. To do this, we need to expand slightly on our discussion of Wiener integrals in Section X.11. Let us do this for general n, rather than $n = 3$. Basic to the construction is the kernel

$$p(x, y; t) = (4\pi t)^{-n/2} e^{-(x-y)^2/4t}$$

of the integral operator e^{-tH_0}. In Section X.11, we constructed a measure μ_x on the continuous paths ω on $[0, \infty)$ with $\omega(0) = x$ so that for $0 < t_1 < \cdots < t_m$,

$$\mu_x\{\omega \,|\, \omega(t_1) \in A_1, \ldots, \omega(t_m) \in A_m\} = \int \prod_{i=1}^m p(x_{i-1}, x_i; t_i - t_{i-1}) \chi_{A_i}(x_i)\, d^n x_i$$

where χ_A is the characteristic function of A and $x_0 = x$, $t_0 = 0$. Because of the semigroup property, μ_x was a measure of total mass 1. By the same method as in X.11, one can construct a measure $\mu_{x,y;t}$ on the continuous paths on $[0, t]$ with $\omega(0) = x$, $\omega(t) = y$ so that for $0 < t_1 < \cdots < t_m < t$,

$$\mu_{x,y;t}\{\omega \,|\, \omega(t_1) \in A_1, \ldots, \omega(t_m) \in A_m\}$$

$$= \int \left(\prod_{i=1}^m p(x_{i-1}, x_i; t_i - t_{i-1}) \chi_{A_i}(x_i) \right) p(x_m, y; t - t_m)\, d^n x_i$$

$\mu_{x,y;t}$ is called **conditional Wiener measure**. It is related to μ_x: For if $f(\omega)$ is a function of the values the path takes on $[0, t]$, then

$$\int f(\omega)\, d\mu_x = \int dy \left[\int f(\omega)\, d\mu_{x,y;t} \right]$$

which is obvious for functions of $\omega(t_1), \ldots, \omega(t_n)$. $d\mu_{x,y;t}$ has total mass $p(x, y; t)$.

The point of conditional Wiener measure is that the Feynman–Kac formula now says that $e^{-t(H_0+W)}$ is an integral operator with kernel

$$e^{-t(H_0+W)}(x, y) = \int d\mu_{x,y;t} \exp\left(-\int_0^t W(\omega(s))\, ds \right) \tag{13}$$

A priori (13) only holds a.e. in x, y; but when $W \in C_0^\infty$, it is not hard to show that the right-hand side of (13) is continuous in x and y (Problem 29). By the basic method used to prove the Feynman–Kac formula, one sees that

$$(e^{-s(H_0+W)}We^{-(t-s)(H_0+W)})(x, y) = \int d\mu_{x,y;t}\, W(\omega(s)) \exp\left(-\int_0^t W(\omega(s))\, ds\right)$$

Using the facts that the kernel on the right-hand side of this expression is continuous and the operator is trace class, one can show that (Problem 30):

$$\mathrm{Tr}(e^{-s(H_0+W)}We^{-(t-s)(H_0+W)})$$

$$= \int dx \int d\mu_{x,x;t}\, W(\omega(s)) \exp\left(-\int_0^t W(\omega(s))\, ds\right)$$

But $\mathrm{Tr}(e^{-s(H_0+W)}W\, e^{-(t-s)(H_0+W)})$ is independent of s by the cyclicity of the trace, so we have that

$$\mathrm{Tr}(We^{-t(H_0+W)}) = \frac{1}{t}\int_0^t \mathrm{Tr}(e^{-s(H_0+W)}W\, e^{-(t-s)(H_0+W)})\, ds$$

$$= \frac{1}{t}\int dx \int d\mu_{x,x;t}\, F\left(\int_0^t W(\omega(s))\, ds\right) \tag{14}$$

where $F(u) = ue^{-u}$.

Armed with (14), we can rewrite the bound (12) as

$$N(V) \leq 2\int_0^\infty dt \int dx \int d\mu_{0,0;t}\, t^{-1} G\left(\int_0^t W(x + \omega(s))\, ds\right) \tag{15}$$

where $G(u) = u(1 - e^{-u})$ and we have used the covariance

$$\int d\mu_{x+a,y+a;t}\, f(\omega(s)) = \int d\mu_{x,y;t}\, f(\omega(s) + a)$$

Now the function G'' is easily seen to be positive on $(0, 2)$ and negative on $(2, \infty)$. Thus, φ given by

$$\varphi(u) = \begin{cases} u(1 - e^{-u}), & 0 < u \leq 2 \\ G(2) + (u-2)G'(2), & 2 \leq u < \infty \end{cases}$$

is easily seen to obey

$$G(u) \leq \varphi(u) \tag{16a}$$

$$\varphi(u) \sim \begin{cases} u^2 & \text{at} \quad u = 0 \\ u & \text{at} \quad u = \infty \end{cases} \tag{16b}$$

$$\varphi(u) \text{ is convex} \tag{16c}$$

$\varphi(u)$ **convex** means that for $u, v \geq 0$, $0 \leq t \leq 1$, $\varphi(tu + (1-t)v) \leq t\varphi(u) + (1-t)\varphi(v)$. This follows from the fact that $\varphi'' \geq 0$. By induction

$$\varphi\left(\sum_{i=1}^{n} t_i u_i\right) \leq \sum_{i=1}^{n} t_i \varphi(u_i)$$

if $\sum t_i = 1$, and $u_i, t_i \geq 0$. By a simple limiting argument, we find that

$$\varphi\left(\int f(x)\, d\mu(x)\right) \leq \int \varphi(f(x))\, d\mu(x) \tag{17}$$

for any positive function f and measure $d\mu$ of total mass 1. On account of (16a) and (17),

$$G\left(\int_0^t W(x + \omega(s))\, ds\right) \leq t^{-1} \int_0^t ds\, \varphi(tW(x + \omega(s)))$$

Using Fubini's theorem, we can thus deduce from (15) that

$$N(V) \leq 2 \int_0^\infty dt\, t^{-2} \int_0^t ds \int d\mu_{0,0;t} \int dx\, \varphi(tW(x + \omega(s)))$$

$$= 2 \int_0^\infty t^{-2}\, dt \int_0^t ds \int d\mu_{0,0;t} \int dx\, \varphi(tW(x))$$

$$= 2 \int_0^\infty (4\pi t)^{-3/2} t^{-1}\, dt \int dx\, \varphi(tW(x))$$

$$= c \int W(x)^{3/2}\, dx$$

where $c = 2(4\pi)^{-3/2} \int_0^\infty u^{-5/2}\varphi(u)$ is finite by (16b). The first equality above follows from the invariance of Lebesgue measure dx; the second from the fact that the integrand is now independent of ω and s and $\int_0^t ds = t$, $\int d\mu_{0,0;t} = p(0, 0, t) = (4\pi t)^{-3/2}$; the third by changing variables from (t, x) to (u, x) with $u = tW(x)$.

This proves the result for $n = 3$. For $n > 3$, this argument fails since $\int_0^\infty u^{-5/2}\varphi(u)$ is replaced by $\int_0^\infty u^{-n/2-1}\varphi(u)$, which diverges at $u = 0$. We introduce the following modifications to overcome this. For any m, we consider the function

$$H_m(y) = \sum_{j=0}^{m} (-1)^j \binom{m}{j} (1 + yj)^{-1}$$

It is useful to note that

$$H_m(y) = m!\, y^m / (1 + y)(1 + 2y) \cdots (1 + my)$$

which follows since the difference of the two functions is an entire function in y, which goes to zero at infinity. By mimicking the argument leading to (11) one obtains

$$N_E(V) \leq (m+1)\,\mathrm{Tr}\left(W\sum_{j=0}^{m}(-1)^j\binom{m}{j}(H_0 + mW + \kappa^2)^{-1}\right) \qquad (11')$$

In proving (11′) the operator K is replaced by

$$K' = W^{1/2}\sum_{j=0}^{m}(-1)^j\binom{m}{j}(H_0 + mW + \kappa^2)^{-1}W^{1/2}$$

$$= W^{1/2}(H_0 + \kappa^2)^{-1/2}H_m(W^{1/2}(H_0 + \kappa^2)^{-1}W^{1/2})(H_0 + \kappa^2)^{-1/2}W^{1/2}$$

which is positive since H_m is. Moreover, $K\psi = (\lambda^{-1} - (1+\lambda)^{-1})\psi$ is replaced by

$$K'\psi = \left(\sum_{j=0}^{m}(-1)^j\binom{m}{j}(j+\lambda)^{-1}\right)\psi = \lambda^{-1}H_m(\lambda^{-1})\psi$$

Since

$$H_m(y) = \int_0^\infty e^{-t}(1 - e^{-yt})^m\,dy$$

it is monotone in y. Thus, as λ goes from 0 to 1, $\lambda^{-1}H_m(\lambda^{-1})$ runs from ∞ to $H(1) = m!/(m+1)! = 1/(m+1)$, so (11′) follows.

Rewriting (11′) in the way we arrived at (15) leads to

$$N(V) \leq (m+1)\int_0^\infty dt \int dx \int d\mu_{0,0;t}\,t^{-1}G_m\left(\int_0^t W(x+\omega(s))\,ds\right)$$

where $G_m(u) = u(1-e^{-u})^m$. G_m'' is seen to be positive on $(0, y_m)$ and negative on (y_m, ∞) for suitable y_m, so φ_m given by

$$\varphi_m(u) = \begin{cases} G_m(u), & 0 < u \leq y_m \\ G_m(y_m) + (u - y_m)G'(y_m), & y_m \leq u < \infty \end{cases}$$

obeys

$$G_m(u) \leq \varphi_m(u)$$

$$\varphi_m(u) \sim \begin{cases} u^{m+1} & \text{at} \quad u = 0 \\ u & \text{at} \quad u = \infty \end{cases}$$

$$\varphi_m(u) \text{ is convex}$$

We then find that for any n, m,

$$N(V) \leq C_{nm}\int W(x)^{m/2}\,d^n x$$

where $C_{nm} = 2(4\pi)^{-n/2} \int_0^\infty u^{-n/2-1}\varphi_m(u)$. So long as $m > (n/2) - 1$, $C_{nm} < \infty$, so choosing m suitably, the theorem is proven for arbitrary $n \geq 3$. ∎

This theorem can also be proven using Theorem XI.22.

XIII.4 Locating the essential spectrum I: Weyl's theorem

In this section and the next we shall discuss methods of determining $\sigma_{\text{ess}}(A)$ for a variety of operators A. In this section we prove a general perturbation theory result that tells us $\sigma_{\text{ess}}(A + C) = \sigma_{\text{ess}}(A)$ if C is compact, or more generally if C is "almost compact" in a sense to be made precise. This will enable us to find σ_{ess} for two-body Schrödinger operators with their center of mass removed. In the next section we shall describe a special theory to deal with the essential spectrum of N-body Schrödinger operators.

We are primarily interested in $\sigma_{\text{ess}}(A)$ when A is self-adjoint, but the natural setting for the results is for a general closed operator. $\sigma_{\text{disc}}(A)$ is defined in Section XII.2 and we define $\sigma_{\text{ess}}(A) = \sigma(A) \backslash \sigma_{\text{disc}}(A)$. The reader is cautioned that many other definitions of σ_{ess} appear in the literature.

The natural way to study $\sigma_{\text{ess}}(A)$ is to study $(A - z)^{-1}$ for some $z \notin \sigma(A)$. For a general self-adjoint operator, it is necessary to take z nonreal, so one is lead to the consideration of non-self-adjoint operators. If one were interested only in semibounded self-adjoint operators, then one could take z to be real and thus deal only with self-adjoint operators. In that case, the proofs below would be slightly simplified.

Our results in this section are based on use of the analytic Fredholm theorem (Theorem VI.14). The proof of our final result will have several complicating features, so let us first prove a very special case of it:

Proposition Let A and B be two bounded self-adjoint operators with empty discrete spectra and with $B - A$ compact. Then $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$.

Proof Write $A = B + C$ with C compact. Define $F(z) = C(A - z)^{-1}$ for $z \in \mathbb{C} \backslash \sigma(A)$. Then $F(z)$ is an analytic operator-valued function of z that is always compact since C is compact by hypothesis. Since A is bounded,

$$\|F(z)\| \leq \|C\| \, \|(A - z)^{-1}\| \to 0$$

in norm as $z \to \infty$. In particular $(1 - F(z))^{-1}$ exists if $|z|$ is large. By the analytic Fredholm theorem, $(1 - F(z))^{-1}$ exists for $z \in \mathbb{C} \backslash (\sigma(A) \cup D)$ where

D is a discrete subset of $\mathbb{C}\backslash\sigma(A)$. Further, $(1 - F(z))^{-1}$ is meromorphic in $\mathbb{C}\backslash\sigma(A)$ with finite rank residues at the points of D. If $z \notin \sigma(A)$, then $B - z = (1 - C(A - z)^{-1})(A - z)$ so if $(1 - F(z))$ is invertible, then $z \notin \sigma(B)$ and $(B - z)^{-1} = (A - z)^{-1}(1 - F(z))^{-1}$. Thus $\sigma(B) \subset D \cup \sigma(A)$. Moreover, $(B - z)^{-1}$ has finite rank residues at the points of D. Thus points of D are in $\sigma_{\text{disc}}(B)$, so $\sigma_{\text{ess}}(B) \subset \sigma(A)$. Similarly, $\sigma_{\text{ess}}(A) \subset \sigma(B)$. By hypothesis, $\sigma_{\text{ess}}(A) = \sigma(A)$ and $\sigma_{\text{ess}}(B) = \sigma(B)$, so we conclude that $\sigma_{\text{ess}}(B) = \sigma_{\text{ess}}(A)$. ∎

We want to extend this proposition in various directions. First we want to allow unbounded operators. Most crucially, we want to eliminate the hypothesis that $\sigma_{\text{disc}}(A) = \varnothing$. To eliminate this last hypothesis, we shall actually require a strengthening of the analytic Fredholm theorem which is of some interest in itself:

Theorem XIII.13 (meromorphic Fredholm theorem) Let Ω be a connected open subset of $\mathbb{C}$. Let $A(z)$ be a meromorphic operator-valued function of z, i.e., A is analytic in $\Omega\backslash D$ where D is a discrete subset of Ω (a set with no limit points *in* Ω) and near any $z_0 \in D$,

$$A(z) = A_{-k}(z - z_0)^{-k} + \cdots + A_{-1}(z - z_0)^{-1} + \sum_{n=0}^{\infty} A_n(z - z_0)^n$$

Suppose in addition that:

(1) $A(z)$ is compact if $z \in \Omega\backslash D$.
(2) The coefficients $A_{-k}, \ldots, A_{-1}$ of the negative terms of the Laurent series of $A(z)$ at points $z_0 \in D$ are finite rank operators.

Then either:

(a) $1 - A(z)$ is invertible for no $z \in \Omega\backslash D$;

or

(b) There is a discrete set $D' \subset \Omega$ so that $(1 - A(z))^{-1}$ exists if $z \notin D \cup D'$ and extends to a function analytic in $\Omega\backslash D'$ and meromorphic in Ω such that the coefficients of the negative terms in the Laurent series at points $z_0 \in D'$ are finite rank operators.

Proof Most of the ideas of the proof are those of Theorem VI.14, so we shall refer to that proof. As in that proof, it is enough to show that any $z_0 \in \Omega$ has a neighborhood N so that either (a) or (b) holds. If $z_0 \in \Omega\backslash D$, the proof that (a) or (b) holds in a neighborhood $N \subset \Omega\backslash D$ is identical to the one in Theorem VI.14. Thus suppose $z_0 \in D$. Near z_0 we know that

$$A(z) = A_{-k}(z - z_0)^{-k} + \cdots + A_{-1}(z - z_0)^{-1} + G(z)$$

where $G(z)$ is analytic at z_0 and compact for z near but not equal to z_0. Since G is norm continuous at z_0, $G(z_0)$ is compact also as a limit of compact operators. Now, let F be a finite rank operator and N be an open disk about z_0, so that $\|G(z_0) - F\| < \frac{1}{2}$ and $\|G(z) - G(z_0)\| < \frac{1}{2}$ if $z \in N$. Let

$$F(z) = A_{-k}(z - z_0)^{-k} + \cdots + A_{-1}(z - z_0)^{-1} + F$$

Then $\|A(z) - F(z)\| < 1$ in N so $C(z) = [1 - (A(z) - F(z))]^{-1}$ exists and is analytic in N. Thus $(1 - A(z))^{-1}$ exists if and only if $[1 - F(z)C(z)]^{-1}$ exists since

$$1 - A(z) = (1 - F(z)C(z))[1 - (A(z) - F(z))]$$

Since $F(z)$ has its range contained in $\operatorname{Ran} A_{-k} + \cdots + \operatorname{Ran} A_{-1} + \operatorname{Ran} F \equiv R$, a fixed finite-dimensional space, $F(z)C(z)$ has its range in R. Thus, by Eq. (VI.5b) of Section VI.5, $1 - F(z)C(z)$ is invertible if and only if a certain determinant of matrix elements of $1 - C(z)F(z)$ is nonzero. This determinant is a meromorphic function in N, and so it has discrete zeros inside N if it is not identically zero. Moreover, in this case $(1 - C(z)F(z))^{-1}$ is given by 1 + finite cofactor matrix/determinant, so $(1 - C(z)F(z))^{-1}$ is meromorphic with finite rank residues in N. Thus we are in case (b) in N. If the determinant is identically zero, we are locally in case (a). ∎

Our condition that the operators $A_{-k}, \ldots, A_{-1}$ be finite rank is crucial. The theorem is false if we only suppose $A_{-k}, \ldots, A_{-1}$ are compact (Problem 34). Theorem XIII.13 provides the technique we need for eliminating the assumption $\sigma(A) = \sigma_{\text{ess}}(A)$ from the above proposition.

Lemma 1 Let A be a closed operator. Then $(A - z)^{-1}$ is a meromorphic function on $\mathbb{C}\backslash\sigma_{\text{ess}}(A)$ with singularities only at points $z \in \sigma_{\text{disc}}(A)$. The negative coefficients of the Laurent expansion at points $z_0 \in \sigma_{\text{disc}}(A)$ are finite rank operators.

Proof We already know that $(A - z)^{-1}$ is analytic in $\mathbb{C}\backslash\sigma(A)$. Let z_0 be an isolated point of $\sigma(A)$. Then $(A - z)^{-1}$ is analytic in a set $\{z | 0 < |z - z_0| < r\}$, and so in that set

$$(A - z)^{-1} = \sum_{n=-\infty}^{\infty} R_n(z - z_0)^n$$

where

$$R_n = (2\pi i)^{-1} \oint_{|z - z_0| = r/2} (z - z_0)^{-n-1}(A - z)^{-1}\, dz$$

In Section XII.2, we used the resolvent identity to prove that $(-R_{-1})^2 = -R_{-1}$. In a similar way one proves (see Problem 3 of Chapter XII) that

$$R_{-n} = -(N)^{n-1} \qquad (n \geq 2) \tag{18a}$$

where $N = -R_{-2}$, and

$$NP = PN = N \tag{18b}$$

where $P = -R_{-1}$ is the projection associated to z_0. Finally, since $\sum_{n=-\infty}^{0} R_n \mu^n$ is absolutely convergent for all $\mu \neq 0$, $\sum_{n=0}^{\infty} \lambda^n N^n$ converges for all λ, so $(1 - \lambda N)^{-1}$ exists for all λ. Thus

$$\sigma(N) = \{0\} \tag{18c}$$

Now suppose that $z_0 \in \sigma_{\text{disc}}(A)$ as well as being isolated. Then P is finite rank by definition. By (18b), Ran $N \subset$ Ran P, so each R_{-n} is finite rank. Moreover, by (18c) $N \restriction$ Ran P is a finite-dimensional operator with spectrum $\{0\}$. Thus $(NP)^k = 0$ for some k. Since $(NP)^k = N^k$ by (18b), $N^k = 0$ for some k. We thus conclude that $R_{-n} = 0$ if $n \geq k + 1$. Thus, $(A - z)^{-1}$ is meromorphic at z_0 with finite rank residues. ∎

We now have the major tools for extending the proposition at the beginning of the section to the case where $\sigma_{\text{disc}}(A) \cup \sigma_{\text{disc}}(B) \neq \varnothing$. The reader might stop at this point and try to use Theorem XIII.13 to extend the proposition in this way. Next, we introduce the tool for extending the proposition to unbounded operators:

Lemma 2 (strong spectral mapping theorem) Let A be a closed operator on a Hilbert space $\mathscr{H}$. Let $z_0 \notin \sigma(A)$ and $B = (A - z_0)^{-1}$. Then:

(a) If $z \neq 0$, then $z \in \sigma(B)$ if and only if $z_0 + z^{-1} \in \sigma(A)$; $z \in \sigma_{\text{ess}}(B)$ if and only if $z^{-1} + z_0 \in \sigma_{\text{ess}}(A)$ and $z \in \sigma_{\text{disc}}(B)$ if and only if $z^{-1} + z_0 \in \sigma_{\text{disc}}(A)$.

(b) $0 \in \sigma(B)$ if and only if A is not bounded. 0 is never in $\sigma_{\text{disc}}(B)$; so if $0 \in \sigma(B)$, then $0 \in \sigma_{\text{ess}}(B)$.

Proof Since we make no use of (b), we leave its proof to the problems (Problem 36). To prove (a), first note that if $z \neq 0$,

$$\begin{aligned} B - z = (A - z_0)^{-1} - z &= [1 - z(A - z_0)](A - z_0)^{-1} \\ &= -z[A - (z^{-1} + z_0)](A - z_0)^{-1} \end{aligned}$$

If $z \notin \sigma(B)$, then $[A - (z^{-1} + z_0)]^{-1} = -z(A - z_0)^{-1}(B - z)^{-1}$ so $z^{-1} + z_0 \notin \sigma(A)$. If $z^{-1} + z_0 \notin \sigma(A)$, then $-z^{-1}(A - z_0)[A - (z^{-1} + z_0)]^{-1} = -z^{-1} - z^{-2}[A - (z^{-1} + z_0)]^{-1}$ is bounded and an inverse for $B - z$, so $z \notin \sigma(B)$. Thus $z \in \sigma(B)$ if and only if $z^{-1} + z_0 \in \sigma(A)$ and isolated points of the spectrum are mapped into one another by $z \mapsto z^{-1} + z_0$. Let $z_1 \in \sigma_{\text{disc}}(B)$. Then near $z = z_1$, $(B - z)^{-1}$ is meromorphic with finite rank residues. Thus for z near z_1, $[A - (z^{-1} + z_0)]^{-1} = -z(A - z_0)^{-1}(B - z)^{-1}$ is meromorphic with finite rank residues. Thus for λ near $z_1^{-1} + z_0$, $(A - \lambda)^{-1}$ is meromorphic with finite rank residues so $z_1^{-1} + z_0 \in \sigma_{\text{disc}}(A)$. Similarly if $\lambda \in \sigma_{\text{disc}}(A)$, one can show $z = (\lambda - z_0)^{-1} \in \sigma_{\text{disc}}(B)$. ∎

If we wanted to state our final theorem only for semibounded self-adjoint operators, we could apply the proposition at the start of this section to $(A + c)^{-1}$ for a suitable real number c. But we want to discuss self-adjoint operators with spectrum $\mathbb{R}$, and we shall need to look at $(A + i)^{-1}$, which is no longer self-adjoint. Thus we need to extend our first proposition to certain bounded non-self-adjoint operators.

The following example shows that it is not necessarily true that $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$ if $B - A$ is compact.

Example 1 Let $\mathscr{H} = \ell_2(-\infty, \infty)$. Let A be the left shift operator, that is, $(A\varphi)_n = \varphi_{n+1}$. Let $C: \mathscr{H} \to \mathscr{H}$ be defined by $(C\varphi)_n = \delta_{n,0}\varphi_1$. Thus C is a rank-one perturbation. Let $B = A - C$. We shall show that $\sigma(A) = \sigma_{\text{ess}}(A) = \{z \,|\, |z| = 1\}$ while $\sigma(B) = \sigma_{\text{ess}}(B) = \{z \,|\, |z| \leq 1\}$. To find $\sigma(A)$ map $\ell_2(-\infty, \infty)$ onto $L^2(0, 2\pi)$ by $U\{\varphi_n\} = \sum_{n=-\infty}^{\infty} (2\pi)^{-1/2}\varphi_n e^{inx}$. Then U is unitary and UAU^{-1} is multiplication by e^{-ix}, so $\sigma(A) = \sigma(UAU^{-1}) = \{z \,|\, |z| = 1\}$. Next we turn to B. If $z \notin \sigma(A)$, then $(B - z)^{-1}$ exists if and only if $(1 - C(A - z)^{-1})^{-1}$ exists. Since $C(A - z)^{-1}$ is compact, $(1 - C(A - z)^{-1})^{-1}$ will exist unless $C(A - z)^{-1}$ has eigenvalue 1 or equivalently if and only if z is an eigenvalue of B. Let $(B - z)\varphi = 0$. Then $\varphi_{n+1} - \delta_{n,0}\varphi_1 - z\varphi_n = 0$. Suppose $z \neq 0$. Letting $n = 0$, we see $\varphi_0 = 0$ and then letting $n = -1, -2, \ldots$ that $\varphi_n = 0$ for $n < 0$. Taking $n = 1, 2, \ldots$ we see $\varphi_n = z^{n-1}\varphi_1$ if $n \geq 1$. Thus if $|z| > 1$, no such eigenvalue exists and $B - z$ is invertible, i.e., $z \in \rho(B)$. If $|z| < 1$,

$$\langle 0, \varphi_1, z\varphi_1, \ldots, z^{n-1}\varphi_1, \ldots \rangle$$

is an eigenvector so $z \in \sigma(B)$.

It is interesting to notice where the proof that $\sigma_{\text{ess}}(B) = \sigma_{\text{ess}}(A)$ breaks down. One still knows $C(A - z)^{-1}$ is analytic in $\mathbb{C}\backslash\sigma(A)$. On the component of $\mathbb{C}\backslash\sigma(A)$ that goes out to infinity, $\|C(A - z)^{-1}\|$ is less than 1 somewhere so

$(1 - C(A - z)^{-1})^{-1}$ exists on that component. On the other component, we do not know a priori that $(1 - C(A - z)^{-1})^{-1}$ exists at any point and so we are in the case (a) of the analytic Fredholm theorem where we obtain little information.

Because of Example 1 we need hypotheses on B that tell us that this situation of everywhere noninvertibility on a component of $\mathbb{C}\backslash\sigma(A)$ does not occur. If we turn Example 1 around, and look at A as a perturbation of B, we see the interior of $\sigma_{ess}(A)$ can disappear under perturbation, so we shall suppose $\sigma_{ess}(A)$ is nowhere dense:

Lemma 3 Let A and B be bounded operators with $A - B$ compact, so that:

(a) $\sigma(A)$ has empty interior as a subset of $\mathbb{C}$.
(b) Each component of $\mathbb{C}\backslash\sigma(A)$ contains a point in $\rho(B)$.

Then $\sigma_{ess}(A) = \sigma_{ess}(B)$.

Proof Let $C = A - B$. Since C is compact, $C(A - z)^{-1}$ is analytic and compact-valued in $\mathbb{C}\backslash\sigma(A)$ and, by Lemma 1, meromorphic in $\mathbb{C}\backslash\sigma_{ess}(A)$ with finite rank residues at points in $\sigma_{disc}(A)$. If $z \notin \sigma(A)$, then $(B - z)^{-1}$ exists if and only if $(1 - C(A - z)^{-1})^{-1}$ exists. Thus, by (b), in each component of $\mathbb{C}\backslash\sigma(A)$ we conclude that $(1 - C(A - z)^{-1})^{-1}$ is invertible somewhere. The components of $\mathbb{C}\backslash\sigma(A)$ and $\mathbb{C}\backslash\sigma_{ess}(A)$ are the same since $\sigma_{disc}(A)$ is discrete. By the meromorphic Fredholm theorem, we conclude that $(1 - C(A - z)^{-1})^{-1}$ exists on $\mathbb{C}\backslash\sigma_{ess}(A)$ except for a discrete set D' where it has finite rank residues. It therefore follows that B can only have discrete spectrum in $\mathbb{C}\backslash\sigma_{ess}(A)$, so $\sigma_{ess}(B) \subset \sigma_{ess}(A)$. Since $\sigma(A)$ has no interior, each component of $\mathbb{C}\backslash\sigma_{ess}(B)$ has a point not in $\sigma(A)$ nor in $\sigma(B)$. We can then turn the above argument around and conclude that $\sigma_{ess}(A) \subset \sigma_{ess}(B)$. ∎

We are now able to prove the main theorem. However, since the basic hypothesis will be that $(A - z)^{-1} - (B - z)^{-1}$ is compact, it is useful to note:

Lemma 4 Let A and B be closed operators. If $(A - z)^{-1} - (B - z)^{-1}$ is compact for some $z_0 \in \rho(A) \cap \rho(B)$, it is compact for all $z \in \rho(A) \cap \rho(B)$.

Proof By using the first resolvent formula, $(A - z)^{-1} - (B - z)^{-1}$ can be written as a finite sum of terms of the form $C[(A - z_0)^{-1} - (B - z_0)^{-1}]D$ with C and D bounded. ∎

We are now ready to prove the main theorem of this section.

Theorem XIII.14 (Weyl's essential spectrum theorem) Let A be a self-adjoint operator and let B be a closed operator so that:

(a) For some (and hence all) $z \in \rho(B) \cap \rho(A)$, $(A - z)^{-1} - (B - z)^{-1}$ is compact

and *either*

(b_1) $\sigma(A) \neq \mathbb{R}$ and $\rho(B) \neq \varnothing$

or

(b_2) There are points of $\rho(B)$ in both the upper and lower half-planes.

Then $\sigma_{ess}(B) = \sigma_{ess}(A)$.

Proof By hypothesis, some z_0 off the real axis is in $\rho(B)$. Let $D = (A - z_0)^{-1}$ and $E = (B - z_0)^{-1}$. By Lemma 2, we need only show $\sigma_{ess}(D) = \sigma_{ess}(E)$ to conclude that $\sigma_{ess}(A) = \sigma_{ess}(B)$. Since A is self-adjoint, $\sigma_{ess}(A) \subset \mathbb{R}$, so $\sigma_{ess}(D) \subset \{\lambda \,|\, \lambda^{-1} + z_0 \in \mathbb{R}\} \cup \{0\}$. As a consequence, $\sigma_{ess}(D)$ has empty interior and either $\sigma_{ess}(A) = \mathbb{R}$ in which case $\mathbb{C}\backslash\sigma_{ess}(D)$ has two components, or $\sigma_{ess}(A) \neq \mathbb{R}$ in which case $\mathbb{C}\backslash\sigma_{ess}(D)$ is connected. In either case, (b) and Lemma 2 imply that each component of $\mathbb{C}\backslash\sigma_{ess}(D)$ intersects $\rho(E)$. Since D and E are bounded with $D - E$ compact by Lemma 4, we can apply Lemma 3 and conclude that $\sigma_{ess}(D) = \sigma_{ess}(E)$. This proves the theorem. ∎

We note that Theorem XIII.14 can be extended to some cases where A is neither self-adjoint nor normal but that the hypotheses are a little complicated. In applications A is almost always self-adjoint, so we stated the theorem in the simple case. The following example shows that some condition of type (b) is needed.

Example 2 Let A and B be the operators of Example 1 so that $\sigma(A) = \{z \,|\, |z| = 1\}$ and $\sigma(B) = \{z \,|\, |z| \leq 1\}$. Notice that 1 is not an eigenvalue of A, A^*, B, or B^* so $A - 1$ and $B - 1$ are injective maps of ℓ_2 onto dense subsets of ℓ_2. Thus $(A - 1)^{-1}$ and $(B - 1)^{-1}$ are unbounded densely defined closed operators. Let $D = i(A + 1)(A - 1)^{-1} = i[1 + 2(A - 1)^{-1}]$ and

$$E = i(B + 1)(B - 1)^{-1} = i[1 + 2(B - 1)^{-1}].$$

Then D is self-adjoint since under the map U discussed in Example 1, D is multiplication by $i(e^{-i\theta} + 1)/(e^{-i\theta} - 1) = -\cot(\theta/2)$. Notice that

$$(D - i)^{-1} = \tfrac{1}{2}A - \tfrac{1}{2}$$

and $(E-i)^{-1} = \frac{1}{2}B - \frac{1}{2}$. Thus, by the strong spectral mapping principle (Lemma 2 above), $\sigma(D) = \mathbb{R}$ and $\sigma(E) = \{z \mid \text{Im } z \leq 0\}$. Moreover, $(D-i)^{-1} - (E-i)^{-1}$ is compact but $\sigma_{\text{ess}}(D) \neq \sigma_{\text{ess}}(E)$. This example is related to Example 1 by using an inverse Cayley transform (see the Notes to Section X.1).

In applying Theorem XIII.14 it is useful to replace (b) with simpler conditions. We thus state two corollaries:

Corollary 1 Let A and B be self-adjoint operators with $(A+i)^{-1} - (B+i)^{-1}$ compact, then

$$\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$$

Proof Since B is self-adjoint, $\rho(B)$ contains points in both half-planes. ∎

To state Corollary 2, we need a new notion:

Definition Let A be self-adjoint. An operator C with $D(A) \subset D(C)$ is called **relatively compact** with respect to A if and only if $C(A+i)^{-1}$ is compact.

We note that if C is relatively compact, then $C(A-z)^{-1}$ is compact for all $z \in \rho(A)$ and that if $C(A-z)^{-1}$ is compact for some $z \in \rho(A)$, then C is relatively compact (Problem 38a). Also relative compactness can be phrased in terms of the Hilbert space $D(A)$ with the norm $\|\varphi\|_A^2 = \|\varphi\|^2 + \|A\varphi\|^2$: C is relatively compact if and only if C is compact as a map from $\langle D(A), \|\cdot\|_A \rangle$ to $\langle \mathscr{H}, \| \ \| \rangle$.

Corollary 2 Let A be a self-adjoint operator and let C be a relatively compact perturbation of A. Then:

(a) $B = A + C$ defined with $D(B) = D(A)$ is a closed operator.
(b) If C is symmetric, B is self-adjoint.
(c) $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$.

Proof $C(A+i\lambda)^{-1} = [C(A+i)^{-1}][(A+i)(A+i\lambda)^{-1}]$ for λ real and positive. If we pass to a spectral representation for A, $(A \pm i)(A \pm i\lambda)^{-1}$ is multiplication by $(x \pm i)(x \pm i\lambda)^{-1}$ so $\text{s-lim}_{\lambda \to \infty} (A \pm i)(A \pm i\lambda)^{-1} = 0$. Since $C(A+i)^{-1}$ is compact, and $[(A+i)(A+i\lambda)^{-1}]^*$ goes strongly to zero, $C(A+i)^{-1}[(A+i)(A+i\lambda)^{-1}]$ goes to zero in norm. Thus

$$\lim \|C(A+i\lambda)^{-1}\| = 0$$

As a result, C is A-bounded with relative bound zero, so (a) and (b) follow immediately (see Section X.2). Moreover, for λ large, both $[1 + C(A + i\lambda)^{-1}]^{-1}$ and $[1 + C(A - i\lambda)^{-1}]^{-1}$ exist, so $(B + i\lambda)^{-1}$ and $(B - i\lambda)^{-1}$ exist for λ large. Thus $\rho(B)$ contains points in each half-plane. Finally, for λ large,

$$(B + i\lambda)^{-1} - (A + i\lambda)^{-1} = (A + i\lambda)^{-1}[(1 + C(A + i\lambda)^{-1})^{-1} - 1]$$
$$= -(B + i\lambda)^{-1}C(A + i\lambda)^{-1}$$

Since $C(A + i\lambda)^{-1}$ is compact, $(B + i\lambda)^{-1} - (A + i\lambda)^{-1}$ is compact, so Theorem XIII.14 is applicable. Thus $\sigma_{\text{ess}}(B) = \sigma_{\text{ess}}(A)$. ∎

There is also a quadratic form version of relative compactness and an analog of Corollary 2 (Problem 39).

By doing some additional work, we can strengthen Corollary 2:

Corollary 3 Let A be a self-adjoint operator and let C be a symmetric operator so that C is a relatively compact perturbation of A^n for some positive integer n. Suppose further that $B = A + C$ is self-adjoint on $D(A)$. Then $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$.

Proof Note that since $D(A) \subset D(C)$, C is A-bounded by the closed graph theorem. Suppose first that $n = 2$. For φ, $\eta \in C^\infty(A)$, $(\varphi, (A^2 + 1)^{-z}C(A^2 + 1)^{-1+z}\eta)$ is analytic in the strip $0 < \text{Re } z < 1$, continuous on the closure, and $C(A^2 + 1)^{-1+iy}$ is compact, so

$$(A^2 + 1)^{-1/2}C(A^2 + 1)^{-1/2}$$

is compact by the lemma below. Thus $(A + i)^{-1}C(A + i)^{-1}$ is compact. Since $D(A) = D(B)$, $(A - i)(B - i)^{-1}$ is a bounded operator, so $(A + C + i)^{-1}C(A + i)^{-1}$ is compact. Because

$$(A + i)^{-1} - (B + i)^{-1} = (B + i)^{-1}C(A + i)^{-1}$$

we can apply Theorem XIII.14 to see that $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$.

We now prove the case of general n by proving that if the hypotheses hold for some $n > 2$, then they hold for $n = 2$. For let φ, $\eta \in C^\infty(A)$. Then

$$(\varphi, C(A^2 + 1)^{-g(z)}\eta)$$

where $g(z) = \frac{1}{2}z + \frac{1}{2}n(1 - z)$, is analytic in the strip $0 < \text{Re } z < 1$ and continuous on the closure. Since $C(A^2 + 1)^{-g(iy)}$ is compact for y real and $C(A^2 + 1)^{-g(1+iy)}$ is bounded, $C(A^2 + 1)^{-g(t)}$ is compact for $t = (n - 2)/(n - 1)$ by the lemma below. Thus C is A^2-compact. ∎

We note that Corollary 3 is false if we require only essential self-adjointness on $D(A)$. For example, suppose that A has compact resolvent and that $C = -A$. Then $\sigma_{ess}(A) = \varnothing$ and $\sigma_{ess}(B) = \{0\}$. In the proof we used:

Lemma Let D be dense in some Hilbert space $\mathscr{H}$ and suppose that for each $z \in S = \{z \mid 0 \leq \text{Re } z \leq 1\}$ we have a quadratic form $a(z)$ on $D \times D$ so that:

(1) $(\eta, a(z)\varphi)$ is analytic in S^{int} and continuous on S for all $\eta, \varphi \in D$.
(2) For $z = iy$ (respectively, $1 + iy$), $a(z)$ is the quadratic form of a compact (respectively, bounded) operator $A(z)$.
(3) $\sup_y \{\|A(iy)\|, \|A(1 + iy)\|\} \equiv M < \infty$.

Then, for any $z \in S^{int}$, $a(z)$ is the quadratic form of a compact operator.

Proof By the Hadamard three lines theorem (see the Appendix to Section IX.4) $|(\eta, a(z)\varphi)| \leq M\|\eta\| \, \|\varphi\|$ for any z, so $a(z)$ is the quadratic form of a bounded operator $A(z)$. The map $z \to A(z)$ is analytic in S^{int} and weakly continuous on S. We must show only that $A(z)$ is compact in S^{int}. We shall give the proof for $z = \frac{1}{2}$; the proof for other z is the same. Let $A = A(\frac{1}{2})$. To show that A is compact, it is sufficient to show that $\| |A|^{1/2}\varphi_n\| \to 0$ as $n \to \infty$ for any orthonormal set $\{\varphi_n\}$. Since $\| |A|^{1/2}\varphi_n \|^2 = (U^*\varphi_n, A\varphi_n)$ for a suitable partial isometry U, we need only show that for any orthonormal set $\{\varphi_n\}$ and any sequence $\{\eta_n\}$ with $\|\eta_n\| \leq 1$, we have $(\eta_n, A\varphi_n) \to 0$ as $n \to \infty$.

Let C be the contour $C_1 \cup C_2 \cup C_3 \cup C_4$ depicted in Figure XIII.2. Then, for any entire function $f(z)$ with $f(\frac{1}{2}) = 1$ we have

$$|(\eta_n, A\varphi_n)| \leq (2\pi)^{-1} \int_C |z - \tfrac{1}{2}|^{-1} |f(z)| \, |(\eta_n, A(z)\varphi_n)| \, |dz|$$

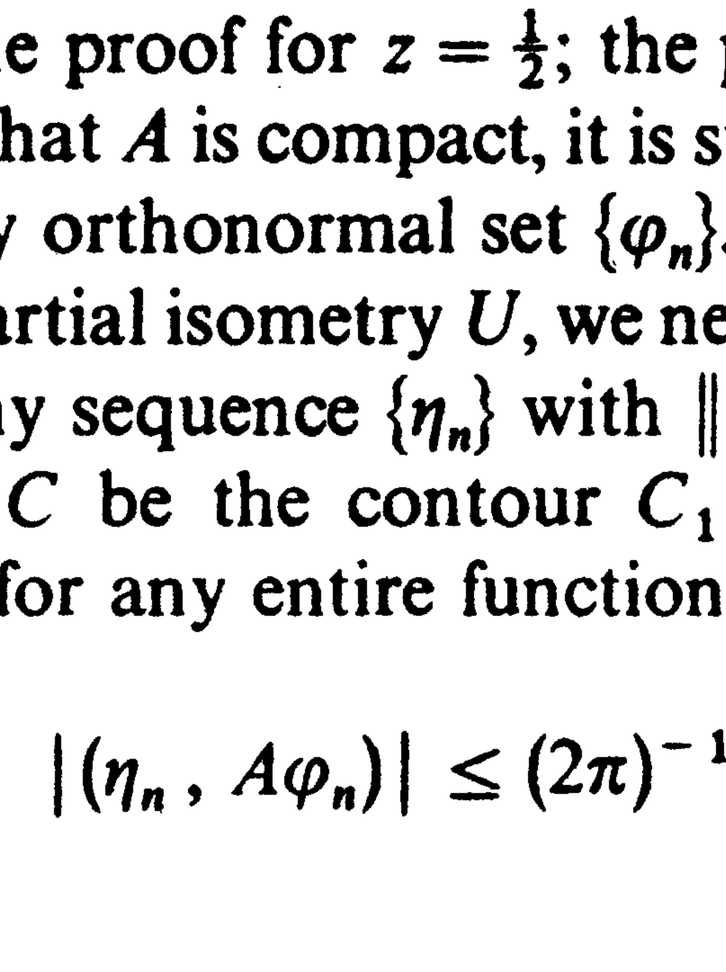


FIGURE XIII.2

Fix $\varepsilon > 0$ and let $f(z) = \exp[z^2 - \frac{1}{4} - B(z - \frac{1}{2})]$. Then $f(\frac{1}{2}) = 1$ and by choosing B and a appropriately we can arrange that

$$(2\pi)^{-1} M \int_{C_2 \cup C_3 \cup C_4} |z - \tfrac{1}{2}|^{-1} |f(z)| \, d|z| \leq \varepsilon$$

But, for each iy on C_1, $\lim_{n\to\infty} |(\eta_n, A(iy)\varphi_n)| = 0$ by the compactness of $A(iy)$. So, since the integrand is uniformly bounded,

$$\lim_{n\to\infty} (2\pi)^{-1} \int_{C_1} |z - \tfrac{1}{2}|^{-1} |f(z)| \, |(\eta_n, A(z)\varphi_n)| \, d|z| = 0$$

by the dominated convergence theorem. Thus, for any $\varepsilon > 0$,

$$\overline{\lim_n} \; |(\eta_n, A\varphi_n)| \leq \varepsilon$$

so $(\eta_n, A\varphi_n) \to 0$ as $n \to \infty$. ∎

There is a quadratic form version of Corollary 3, which is often useful:

Corollary 4 Let A be a positive self-adjoint operator and let C be a self-adjoint operator with $Q(C) \supset Q(A)$. Suppose that the sum of quadratic forms $A + C$ is bounded from below and closed on $Q(A)$ and let B be the corresponding self-adjoint operator. Suppose further that *either*:

(i) C is a relatively compact perturbation of A^n for some positive integer n;

or

(ii) $Q(|C|) \supset Q(A)$ and $|C|$ is a relatively form-compact perturbation of A^n for some positive integer n, i.e., $(A + 1)^{-n/2}|C|(A + 1)^{-n/2}$ is compact.

Then $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$.

Proof As in the case of Corollary 3, it suffices to prove that $(A + \lambda)^{-1}C(B + \lambda)^{-1}$ is compact where $\lambda > 0$ is chosen with $-\lambda < \inf \sigma(B)$. Writing

$$(A + \lambda)^{-1}C(B + \lambda)^{-1} = [(A + \lambda)^{-1}C(A + \lambda)^{-1/2}][(A + \lambda)^{+1/2}(B + \lambda)^{-1/2}] \times (B + \lambda)^{-1/2}$$

and noting that, since $Q(A) = Q(B)$, $(A + \lambda)^{1/2}(B + \lambda)^{-1/2}$ is bounded, we conclude that it suffices to prove that $(A + 1)^{-1}C(A + 1)^{-1/2}$ is compact. Under hypothesis (i), this follows by interpolating between the fact that $(A + 1)^{-n}C(A + 1)^{-1/2}$ is compact and that $(A + 1)^{-1/2}C(A + 1)^{-1/2}$ is bounded. Under hypothesis (ii), we note that $|C|^{1/2}(A + 1)^{-1/2}$ is bounded

and $|C|^{1/2}(A-1)^{-n/2}$ is compact, so by interpolation, $|C|^{1/2}(A+1)^{-1}$ is compact. Thus

$$(A+1)^{-1}C(A+1)^{-1/2} = [|C|^{1/2}(A+1)^{-1}]^*(\operatorname{sgn} C)[|C|^{1/2}(A+1)^{-1/2}]$$

is compact. ∎

We are now ready to consider various examples where Weyl's theorem is applicable:

Example 3 (classical Weyl theorem) If A is self-adjoint and C is compact, then $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(A+C)$. This holds because C is automatically relatively compact.

Example 4 Let $V \in C_0^\infty(0,\infty)$ and let H be the operator $-d^2/dx^2 + V$ on $C_0^\infty(0,\infty)$. H is not self-adjoint but it has deficiency indices $\langle 1,1\rangle$ (see the Appendix to Section X.1). Let A and B be two different self-adjoint extensions of H. If $D = D(\bar{H})$, then $\operatorname{Ran}(\bar{H}+i) \equiv R$ is a closed subspace codimension 1 since H has deficiency indices $\langle 1,1\rangle$. If $\psi \in R$, then $\psi = (\bar{H}+i)\varphi$ for some φ and thus

$$[(A+i)^{-1} - (B+i)^{-1}]\psi = (A+i)^{-1}(\bar{H}+i)\varphi - (B+i)^{-1}(\bar{H}+i)\varphi = 0$$

since $\bar{H} \subset A$ and $\bar{H} \subset B$. Thus $(A+i)^{-1} - (B+i)^{-1}$ vanishes on R. Since R has codimension 1, it follows that $(A+i)^{-1} - (B+i)^{-1}$ is rank 1 and so compact. Thus $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$.

Example 5 In general, let H be an operator with deficiency indices $\langle d,d\rangle$ with $d < \infty$. If A and B are two self-adjoint extensions of H, then $(A+i)^{-1} - (B+i)^{-1}$ is a rank d operator as in Example 4 so $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$. If $d = \infty$, the conclusion need not hold (Problem 40).

Example 6 Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$. By using the Fourier transform one can easily see that $\sigma_{\text{ess}}(-\Delta) = [0,\infty)$. Let V be in $L^2 + (L^\infty)_\varepsilon$; then $V(H_0+1)^{-1}$ is compact. For, we can find $V_n \in L^2$ with $V - V_n \in L^\infty$ and $\lim_{n\to\infty} \|V_n - V\|_\infty = 0$. Thus $V_n(H_0+1)^{-1}$ converges in norm to $V(H_0+1)^{-1}$, so we need only show that $V_n(H_0+1)^{-1}$ is compact for each n. But $V_n(H_0+1)^{-1}$ is an integral operator with kernel $V_n(x)e^{-|x-y|}/4\pi|x-y|$, which is in $L^2(\mathbb{R}^6)$. Thus $V_n(H_0+1)^{-1}$ is Hilbert–Schmidt and so compact. Since $V(H_0+1)^{-1}$ is compact, V is relatively compact and so $\sigma_{\text{ess}}(-\Delta+V) = \sigma_{\text{ess}}(-\Delta) = [0,\infty)$.

For an extension of this result to n-dimensions ($n \neq 3$), see Problem 41

Example 7 More generally, let $V \in R + (L^\infty)_\varepsilon$. In general V is not relatively compact since $D(V)$ may not contain $D(H_0)$. However, it is a form-compact perturbation and so the theory of Problem 39 can be used. Instead, we note that if $W \in R$, then

$$\lim_{E \to +\infty} \| \, |W|^{1/2}(H_0 + E)^{-1} |W|^{1/2} \| = 0$$

since $|W|^{1/2}(H_0 + E)^{-1}|W|^{1/2}$ is a Hilbert–Schmidt operator with kernel

$$|W(x)|^{1/2} \exp(-\sqrt{E}\,|x - y|)|W(y)|^{1/2}/4\pi|x - y|$$

and this kernel has L^2-norm going to 0 by the dominated convergence theorem. Thus, for E large and positive

$$(H + E)^{-1} - (H_0 + E)^{-1}$$

$$= \sum_{n=0}^{\infty} ((H_0 + E)^{-1}|W|^{1/2})[-W^{1/2}(H_0 + E)^{-1}|W|^{1/2}]^n (W^{1/2}(H_0 + E)^{-1})$$

where $H = H_0 + W$ and $W^{1/2} \equiv W/|W|^{1/2}$. Each term in this norm convergent sum is compact. For, letting $A = (H_0 + E)^{-1/2}|W|^{1/2}$, A^*A is compact, and so A is compact. Thus if $W \in R$, then $(H_0 + W + E)^{-1} - (H_0 + E)^{-1}$ is compact. The extension from R to $R + (L^\infty)_\varepsilon$ is as above.

Example 8 Consider the operator $H \equiv -\Delta + \mathbf{a} \cdot \mathbf{x} + V(x)$ associated to the Stark effect problem. By Theorem X.29 and Theorem X.38, we know that H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ if $V \in L^p(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$ where $p = 2$ if $n \leq 3$, $p > 2$ if $n = 4$ and $p = n/2$ if $n \geq 5$. Because the $\mathbf{a} \cdot \mathbf{x}$ term tends to $-\infty$ in a way that cannot be compensated for by the $-\Delta$, one can show that H is not bounded below and one expects that $\sigma(H) = (-\infty, \infty)$. Under the stronger hypothesis that $V = V_1 + V_2$ with $V_1 \in L^p$ having compact support and $V_2 \in L^\infty$ going to zero at infinity, we shall show that V is a relatively compact perturbation of $H_0 = -\Delta + \mathbf{a} \cdot \mathbf{x}$. Let p_a be the momentum operator in the direction parallel to $\mathbf{a}$ and $p_a^\perp$ the momentum orthogonal. Then on $\mathscr{S}(\mathbb{R}^n)$, an elementary calculation (see Section XI.4) shows that

$$\exp(-i\alpha p_a^3) H_0 \exp(+i\alpha p_a^3) = (p_a^\perp)^2 + \mathbf{a} \cdot \mathbf{x} \equiv \tilde{H}_0$$

where $\alpha = (3|a|)^{-1}$. $\tilde{H}_0$ can be "diagonalized" by Fourier transforming in the directions orthogonal to $\mathbf{a}$. It follows that H_0 is essentially self-adjoint on $\mathscr{S}(\mathbb{R}^n)$ and $\sigma(H_0) = (-\infty, \infty)$ so that if V is relatively compact, we have a new proof that $H_0 + V$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R}^n)$ and moreover that $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0) = (-\infty, \infty)$, so that $\sigma(H) = (-\infty, \infty)$. As above,

the V_2 part of V is easy to add if we show that $V_1(H_0 + i)^{-1}$ is compact. Let $T = -\Delta$. Then on $\mathscr{S}$ which is a core for both H_0 and T,

$$\begin{aligned}(H_0 + i)^{-1} &= (T + i)^{-1} - (T + i)^{-1}(\mathbf{a} \cdot \mathbf{x})(H_0 + i)^{-1} \\ &= (T + i)^{-1} - (\mathbf{a} \cdot \mathbf{x})(T + i)^{-1}(H_0 + i)^{-1} \\ &\quad + 2i|a|(T + i)^{-1}p_a(T + i)^{-1}(H_0 + i)^{-1}\end{aligned}$$

because $[\mathbf{a} \cdot \mathbf{x}, T] = 2i|a|p_a$. Since V_1 and $(\mathbf{a} \cdot \mathbf{x})V_1$ are relatively compact perturbations of T (Problem 41) and $p_a(T + i)^{-1}$ is bounded, $V_1(H_0 + i)^{-1}$ is compact.

We summarize the above results together with Problem 41:

Theorem XIII.15 Let $H = -\Delta + \mathbf{a} \cdot \mathbf{x} + V$ on $L^2(\mathbb{R}^n)$. Then:

(a) If $a = 0$, $n = 3$, $V \in R + L^\infty_\varepsilon$, then $\sigma_{\text{ess}}(H) = [0, \infty)$.
(b) If $a = 0$, $V \in L^p + L^\infty_\varepsilon$ where $p \geq \max\{n/2, 2\}$ if $n \neq 4$, $p > 2$ if $n = 4$, then $\sigma_{\text{ess}}(H) = [0, \infty)$
(c) If $a \neq 0$, $V = V_1 + V_2$ where $V_1 \in L^p$ (p as above) has compact support and $V_2 \in L^\infty$ goes to zero at infinity, then $\sigma(H) = \sigma_{\text{ess}}(H) = (-\infty, \infty)$.

Using Corollary 4, certain other potentials can be handled.

Example 9 Let $V = |r|^{-2}$ on $L^2(\mathbb{R}^5)$ and let $H_0 = -\Delta$. Then V cannot be H_0-compact since it does not have relative bound zero (see Example 4 in Section X.2). However, by the following general criterion, V is H_0^2-compact.

Suppose that $V \in L^2(\mathbb{R}^5) + (L^\infty(\mathbb{R}^5))_\varepsilon$. Then for each $\varepsilon > 0$ we may write $V = V_{1,\varepsilon} + V_{2,\varepsilon}$ where $V_{1,\varepsilon} \in L^2$ and $\sup_x |V_{2,\varepsilon}(x)| \leq \varepsilon$. Thus, $V_{1,\varepsilon}(H_0^2 + 1)^{-1}$ converges in norm to $V(H_0^2 + 1)^{-1}$, so we need only show that $V_{1,\varepsilon}(H_0^2 + 1)^{-1}$ is compact for each $\varepsilon > 0$. But this is immediate since $V_{1,\varepsilon} \in L^2$ and $(p^4 + 1)^{-1} \in L^2$ imply that $V_{1,\varepsilon}(H_0^2 + 1)^{-1}$ is Hilbert–Schmidt.

Returning to the case $V = |r|^{-2}$, we see from Example 4 of Section X.2 that if $\lambda \geq -2.25$, then $Q(-\Delta + \lambda V) = Q(-\Delta)$ and $-\Delta + \lambda V$ is bounded from below. For such λ, Corollary 4 is applicable, so $\sigma_{\text{ess}}(-\Delta + \lambda V) = [0, \infty)$. Similar considerations apply to the case $V = |r|^{-1}$ when $H_0 = \sqrt{-\Delta + m^2}$. When H_0 is a Dirac operator, H_0 is not bounded from below, so more subtle methods are needed.

Theorem XIII.15 shows that if V is a bounded function of compact support on $\mathbb{R}^3$, then $-\Delta + V$ has only finitely many eigenvalues in $(-\infty, -1]$. And, it is not hard to extend this to $\mathbb{R}^n$ (Problem 41). It can be proven

(indeed when $n \geq 3$ we have already proven in Theorem XIII.12) that there are only finitely many eigenvalues in $(-\infty, 0)$, but the simpler $(-\infty, -1]$ result suffices for the following application:

Theorem XIII.16 Let V be a locally bounded positive function with $V(x) \to \infty$ as $|x| \to \infty$. Define $-\Delta + V$ as a sum of quadratic forms. Then $-\Delta + V$ has purely discrete spectrum.

Proof Let $H = -\Delta + V$. By the min–max principle, it suffices to prove that $\mu_n(H) \to \infty$ as $n \to \infty$. Given c, find a ball S with $V(x) \geq c$ if $x \notin S$. Such a ball exists since $V(x) \to \infty$ as $x \to \infty$. Let W be the potential that is $-c$ if $x \in S$ and 0 if $x \notin S$. Then $V \geq c + W$ so that

$$\mu_n(H) \geq c + \mu_n(-\Delta + W)$$

Since W is a bounded potential of compact support, there is an N with $\mu_n(-\Delta + W) \geq -1$ if $n \geq N$. Thus $\mu_n(H) \geq c - 1$ if $n \geq N$. Since c was arbitrary, $\mu_n(H) \to \infty$ as $n \to \infty$. ∎

We shall return to the general question of operators with purely discrete spectra in Sections 14 and 15.

XIII.5 Locating the essential spectrum II: The HVZ theorem

The Weyl theorem suffices to prove that $\sigma_{\text{ess}}(-\Delta + V) = [0, \infty)$ for a large class of two body Schrödinger operators. In this section we analyze the spectrum of N-body Schrödinger operators of the type discussed in Section XI.5. We use without comment the notation introduced there.

In the two-body case a key role was played by the condition that $V(\mathbf{x})$ go to zero at infinity at least in the average sense implied by $V \in R + (L^\infty)_\varepsilon$. In the N-body case this is no longer true. Even if V_{ij} is in C_0^∞, $V = \sum_{i<j} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$ fails to go to zero at infinity in tubes where $\sum_{i=1}^{n-1} |\mathbf{r}_i - \mathbf{r}_n|^2 \to \infty$ while some $|\mathbf{r}_i - \mathbf{r}_j|$ remains finite. This is reflected in the technical fact that $(H_0 + I)^{-1}V$ is not compact. The important new idea will be to replace

$$(H - E)^{-1} = (H_0 - E)^{-1} - (H_0 - E)^{-1}V(H - E)^{-1}$$

with an equation

$$(H - E)^{-1} = D(E) + I(E)(H - E)^{-1}$$

where $I(E)$ is compact.

We will give two distinct proofs of the basic result of this section. The first, based on Lemmas 1–6, uses resolvent equations of the type just discussed. The second, using Lemmas 1, 2, and 7–11 is based on geometric ideas of the type indicated above when we discussed the special tubes in which V fails to go to zero. Each proof has its advantages: the first is especially appropriate in cases where H is not self-adjoint such as the situation arising in Sections 10 and 11. As we shall see below, the second proof is particularly convenient when H is restricted to an invariant subspace.

For each cluster decomposition $D = \{C_\ell\}_{\ell=1}^k$ of $\{1, \ldots, n\}$, we defined in Section XI.5 a Hamiltonian $H_D = H - I_D$ where I_D is the sum of all potentials V_{ij} with i and j in different clusters. For potentials $V_{ij} \in L^2 + L^p$ $(p < 3)$, we proved that $\sigma(H_D) \subset \sigma(H)$ since the wave operators $\Omega_D^\pm$ provide a unitary equivalence of H_D and $H \restriction \operatorname{Ran} \Omega_D^\pm$. To find $\sigma(H_D)$, we write $\mathscr{H} = \mathscr{H}(C_1) \otimes \cdots \otimes \mathscr{H}(C_k) \otimes \mathscr{H}_D$ corresponding to the breakup of $\mathscr{H}$ resulting from choosing internal coordinates $\xi_1^{(C_1)}, \ldots, \xi_{n_1-1}^{(C_1)}$ for $C_1, \ldots, \xi_1^{(C_k)}, \ldots, \xi_{n_k-1}^{(C_k)}$ for C_k and $\zeta_1, \ldots, \zeta_{k-1}$ for the relative coordinates of the clusters. Then

$$H_D = H(C_1) + \cdots + H(C_k) + T_D$$

where

$$H(C_\ell) = I \otimes \cdots \otimes h_{C_\ell} \otimes \cdots \otimes I$$

is the Hamiltonian of cluster C_ℓ with its center of mass removed and T_D is the kinetic energy of the clusters, i.e., the sum of the kinetic energies of the centers of mass of the C_ℓ minus the kinetic energy of the center of mass of the entire system. Thus by Theorem VIII.33,

$$\sigma(H_D) = \left\{ \sum_{\ell=1}^k \lambda_\ell + \tau \,\middle|\, \lambda_\ell \in \sigma(H(C_\ell)),\ \tau \in \sigma(T_D) \right\}$$

Since $\sigma(T_D) = [0, \infty)$, we have $\sigma(H_D) = [\Sigma_D, \infty)$, where

$$\Sigma_D = \sum_{\ell=1}^k \inf \sigma(H(C_\ell)) \tag{19}$$

Since we expect that $\mathscr{H}$ should consist only of bound states and scattering states, we expect that $\sigma_{\text{ess}}(H) = [\Sigma, \infty)$ where

$$\Sigma = \inf_{D,\ \#(D) \geq 2} \Sigma_D \tag{20a}$$

In fact, this is true under much more general conditions than $V \in L^2 + L^p$.

Theorem XIII.17 (the HVZ theorem) Let H be the operator on $L^2(\mathbb{R}^{3N-3})$ obtained by removing the center of mass motion from

$$-\sum_{i=1}^N (2\mu_i)^{-1} \Delta_i + \sum_{i<j} V_{ij}(\mathbf{r}_{ij}), \quad \text{where} \quad V_{ij} \in R + (L^\infty)_\varepsilon, \quad \text{and} \quad \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$$

For each cluster decomposition $D = \{C_1, \ldots, C_k\}$, define Σ by (19) and (20a). Then

$$\sigma_{\text{ess}}(H) = [\Sigma, \infty)$$

The remainder of this section is concerned with the proof of the HVZ theorem. The techniques that we develop are useful in the study of many aspects of N-body systems with more than one channel, i.e., systems for which some H_D possesses a bound state. In particular, these techniques play an important role in Section 10. Before proving this theorem, we note that it follows inductively that $\inf\{\Sigma_D \mid \#(D) = m + 1\} \geq \inf\{\Sigma_D \mid \#(D) = m\}$, so (20a) can be replaced by (Problem 42):

$$\Sigma = \inf\{\Sigma_D \mid \#(D) = 2\} \tag{20b}$$

We shall show that $[\Sigma, \infty) \subset \sigma(H)$ by first assuming that the V_{ij} are nice and then using an approximation argument.

Lemma 1 If $V_{ij} \in C_0^\infty(\mathbb{R}^3)$, then $[\Sigma, \infty) \subset \sigma(H)$.

Proof Since the wave operators $\Omega_D^\pm$ exist (Theorem XI.34), $\sigma(H_D) \subset \sigma(H)$. Since $\sigma(H_D) = [\Sigma_D, \infty)$ if $\#(D) \geq 2$, the result holds. ∎

For an alternative proof of Lemma 1, avoiding the use of wave operators, see Problem 45.

Lemma 2 Under the hypotheses of Theorem XIII.17, $[\Sigma, \infty) \subset \sigma(H)$.

Proof For each i, j, we can find $V_{ij}^{(n)} \in C_0^\infty$ so that, as forms, $|V_{ij} - V_{ij}^{(n)}| \leq n^{-1}(-\Delta + 1)$ (Problem 44). Letting $H^{(n)} = H_0 + \sum_{i<j} V_{ij}^{(n)}$ we see that $H^{(n)} \to H$ in norm resolvent sense and that $H_D^{(n)} \to H_D$ similarly. Thus, by Theorem VIII.20, $\exp(-H_D^{(n)}) \to \exp(-H_D)$ in norm. Since $\Sigma_D^{(n)} = -\log\|e^{-H_D^{(n)}}\|$, we conclude that $\Sigma_D^{(n)} \to \Sigma_D$ and thus $\Sigma^{(n)} \to \Sigma$. Let $\lambda > \Sigma$. For n sufficiently large, we conclude that $\lambda > \Sigma^{(n)}$, so $\lambda \in \sigma(H^{(n)})$ by Lemma 1. Since $H^{(n)} \to H$ in norm resolvent sense, $\lambda \in \sigma(H)$ by Theorem VIII.23. Thus $(\Sigma, \infty) \subset \sigma(H)$. Since $\sigma(H)$ is closed, $\Sigma \in \sigma(H)$. ∎

The proof of the other direction of Theorem XIII.17, namely that if $\lambda < \Sigma$, then either $\lambda \in \sigma_{\text{disc}}(H)$ or $\lambda \in \rho(H)$, is considerably harder than Lemma 2 and requires the development of some machinery. To illustrate the ideas, let us first discuss the case where $N = 3$ and $V_{ij} \in L^2$. In the two-body case, we used the key equation $(H - E)^{-1} = (H_0 - E)^{-1} - (H_0 - E)^{-1} V (H - E)^{-1}$

and the critical fact that $(H_0 - E)^{-1}V$ is compact. In the three-body case we still have

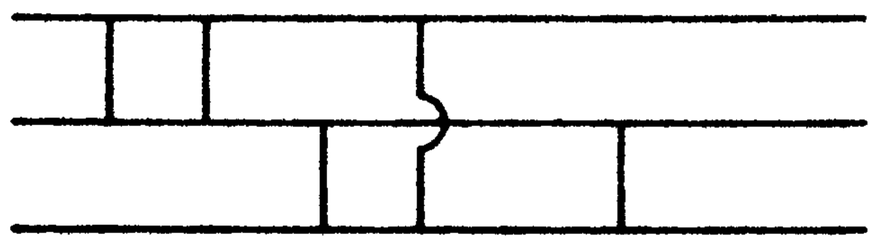
$$(H - E)^{-1} = (H_0 - E)^{-1} - (H_0 - E)^{-1}(V_{12} + V_{13} + V_{23})(H - E)^{-1}$$

but it is no longer true that $(H_0 - E)^{-1}(V_{12} + V_{13} + V_{23})$ is compact. To see that $(H_0 - E)^{-1}V_{12}$ is not compact, notice that it commutes with the one-parameter group of translations $\langle r_1, r_2, r_3\rangle \mapsto \langle r_1 - a, r_2 - a, r_3\rangle$. Such an operator cannot be compact (see Problem 43).

Thus we seek a decomposition of $(H - E)^{-1}$ into the form $A(E) + B(E) \times (H - E)^{-1}$ with $B(E)$ compact, which must be more subtle than the decomposition given by the second resolvent equation. To get an idea for the proper decomposition take E so negative that the perturbation series obtained by iterating the second resolvent equation converges. Then

$$\begin{aligned}(H - E)^{-1} = (H_0 - E)^{-1} &- (H_0 - E)^{-1}V_{12}(H_0 - E)^{-1} \\ &- (H_0 - E)^{-1}V_{13}(H_0 - E)^{-1} \\ &- (H_0 - E)^{-1}V_{23}(H_0 - E)^{-1} \\ &+ (H_0 - E)^{-1}V_{12}(H_0 - E)^{-1}V_{12}(H_0 - E)^{-1} + \cdots \quad (21)\end{aligned}$$

We introduce a graphical notation for individual terms in (21). $\equiv$ represents a factor of $(H_0 - E)^{-1}$ and a vertical line joining lines i and j represents a factor of $-V_{ij}$. Thus, the diagram



represents the operator

$$\begin{aligned}(-1)^5&(H_0 - E)^{-1}V_{12}(H_0 - E)^{-1}V_{12}(H_0 - E)^{-1}V_{23}(H_0 - E)^{-1} \\ &\times V_{13}(H_0 - E)^{-1}V_{23}(H_0 - E)^{-1}\end{aligned}$$

In terms of diagrams, it is easy to describe which terms in (21) are compact:

Lemma 3A A diagram represents a compact operator if and only if it is connected. In fact, if a diagram G is connected and if the last factor of $(H_0 - E)^{-1}$ is removed, then the operator remains compact.

Proof We remark that we are interpreting the symbol $(H_0 - E)^{-1}V_{ij}$ as the (bounded) closure of the operator defined on $D(H_0)$ or alternatively as the adjoint of the everywhere defined operator $V_{ij}(H_0 - \bar{E})^{-1}$. If a diagram is disconnected, by relabeling the particles we can suppose that line 3 is not

linked to lines 1 and 2. Then the associated operator commutes with the unitary operator induced by the map $\langle r_1, r_2, r_3\rangle \mapsto \langle r_1 + a, r_2 + a, r_3\rangle$, so the operator is not compact (Problem 43).

On the other hand, if G is connected, it must contain two consecutive links that are different. By relabeling, we may suppose they are V_{12} and V_{23}. The operator associated with G after the last $(H_0 - E)^{-1}$ removed is then of the form $A[(H_0 - E)^{-1}V_{12}(H_0 - E)^{-1}V_{23}]B$ where A and B are products of terms of the form $(H_0 - E)^{-1}V_{ij}$. Since A and B are bounded, we need only prove that $C = (H_0 - E)^{-1}V_{12}(H_0 - E)^{-1}V_{23}$ is compact. Let us work in momentum space with momentum variables p, q representing the relative momenta of 1 to 2 and 2 to 3, i.e., we consider the operator $D = \mathscr{F}C\mathscr{F}^{-1}$ where $\mathscr{F}$ is the Fourier transform, in terms of the variables $\langle p, q\rangle$ dual to $\langle r_{12}, r_{23}\rangle$. Let $h_0(p, q)$ be the kinetic energy written in terms of p and q. Explicitly,

$$h_0(p, q) = (2m_{12})^{-1}p^2 + (2m_{23})^{-1}q^2 - \mu_2^{-1}p \cdot q$$

where $m_{ij}^{-1} = \mu_i^{-1} + \mu_j^{-1}$. Then

$$(D\psi)(p, q) = (2\pi)^{-3} \int (h_0(p, q) - E)^{-1}\hat{V}_{12}(p - p')$$

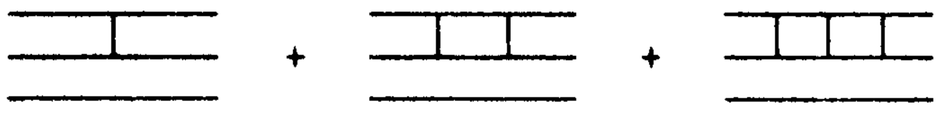
$$\times (h_0(p', q) - E)^{-1}\hat{V}_{23}(q - q')\psi(p', q')\, dp'\, dq' \qquad (22)$$

Since E is negative, $|h_0(p, q) - E| > c(p^2 + q^2 + 1)$ for some constant c. Thus the kernel in (22) is bounded by

$$(2\pi)^{-3}c^{-2}(p^2 + 1)^{-1}\hat{V}_{12}(p - p')(q^2 + 1)^{-1}\hat{V}_{23}(q - q')$$

Since $\hat{V}_{12}, \hat{V}_{23} \in L^2$, this kernel is in $L^2(\mathbb{R}^{12})$ and so the integral operator in (22) is Hilbert–Schmidt. Therefore D and C are compact. ∎

This suggests that in attempting to find an expansion $(H - E)^{-1} = A(E) + B(E)(H - E)^{-1}$ with $B(E)$ compact, we should choose $A(E)$ to be the sum of all disconnected diagrams in the formal expansion (21) when E is negative and then determine $A(E)$ by analytic continuation to other E. To make this continuation, we need a closed expression for this sum of disconnected diagrams. The disconnected diagrams fall naturally into four classes according to whether no horizontal lines are connected to each other or whether only one of the three pairs is connected to each other. Only $\equiv = (H_0 - E)^{-1}$ is in the first class. The class where 1 and 2 are connected together has a sum



(23)

If we add $\equiv$ to this sum, we obtain the sum of all graphs for the case with $V_{23} = V_{13} = 0$. Thus, the sum (23) is $(H_0 + V_{12} - E)^{-1} - (H_0 - E)^{-1}$. Introducing the notation

$$G_0(E) = (H_0 - E)^{-1}$$

$$G_{ij}(E) = (H_0 + V_{ij} - E)^{-1}$$

$$G(E) = (H_0 + V - E)^{-1}$$

We can rewrite (23) as $-G_{12}(E)V_{12}G_0(E)$. This suggests:

Definition Let $E \notin [\Sigma, \infty)$ be a complex number. The **disconnected part of the resolvent** or, for short, the **disconnected part** is defined by

$$D(E) = G_0(E) - \sum_{1 \le i < j \le 3} G_{ij}(E)V_{ij}G_0(E) \tag{24a}$$

Similarly, we can analyze the connected diagrams. A diagram is called **barely connected** if it becomes disconnected when its last leg is removed. The sum of the barely connected diagrams falls into six parts, one of which is



and the other classes are obtained by permuting the labels 1, 2, 3. Each connected diagram can be broken at a unique point in such a way that a barely connected diagram occurs to the left of the break. We can obtain all connected diagrams by placing an arbitrary barely connected diagram to the left of the break and an arbitrary diagram to the right. Thus, formally

$$\begin{aligned}\sum(\text{all connected diagrams}) = (&\sum(\text{all barely connected diagrams}\\ &\text{with the final } G_0(E) \text{ removed}))\\ &\times(\sum(\text{all diagrams}))\end{aligned}$$

if we do not distinguish a diagram and its associated operator. We have used the symbol $\sum(\ )$ to denote the sum of all diagrams with property $(\ )$ in the formal expansion (21). Since $\sum$ (all diagrams) is $(H - E)^{-1}$, we seek a closed expression for the first factor. The sum associated with the class of barely connected diagrams drawn above is clearly

$$-[G_{12}(E) - G_0(E)]V_{23} = G_{12}(E)V_{12}G_0(E)V_{23}$$

Definition Let $E \notin [\Sigma, \infty)$ be a complex number. The **Weinberg connected interaction** or **Weinberg kernel** is defined by

$$I(E) = \sum_{\substack{j \neq k \neq i \\ i < j}} G_{ij}(E)V_{ij}G_0(E)(V_{jk} + V_{ik}) \tag{24b}$$

We are now prepared for:

Lemma 4A The functions $D(E)$ and $I(E)$ are analytic operator-valued functions in the region $\mathbb{C}\backslash[\Sigma, \infty)$. If $E \notin \sigma(H)$, then

$$(H - E)^{-1} = D(E) + I(E)(H - E)^{-1} \tag{24c}$$

Moreover, $I(E)$ is compact for all $E \in \mathbb{C}\backslash[\Sigma, \infty)$, and $\lim_{E \to -\infty} \|I(E)\| = 0$. (24) is called the **Weinberg–Van Winter equation**.

Proof Since $\mathbb{C}\backslash[\Sigma, \infty) \subset \bigcup_{i<j} \rho(H_0 + V_{ij})$, $D(E)$ and $I(E)$ are analytic if we interpret $G_0(E)V_{ij}$ as the adjoint of the bounded operator $V_{ij}G_0(E)^*$ and similarly for $G_{ij}(E)V_{kl}$. Choose E so negative that the perturbation series (21) converges absolutely in operator norm. Then we can rearrange sums of diagrams at will and see that (24c) holds. By analytic continuation, (24c) extends to any $E \notin \sigma(H) \cup [\Sigma, \infty)$ which is equal to $\sigma(H)$ by Lemma 2. Since $\|G_0(E)V_{ij}\| \to 0$ as $E \to -\infty$, $\lim_{E \to -\infty} \|I(E)\| = 0$. Finally, we notice that if E is so negative that the perturbation series for $I(E)$ converges, $I(E)$ is compact by Lemma 3A and the basic fact that the compact operators are norm closed (Theorem VI.12a). That $I(E)$ is compact for all $E \in \mathbb{C}\backslash[\Sigma, \infty)$ follows from Lemma 5 below. ∎

Lemma 5 Let $f(z)$ be an operator-valued function on a connected region $R \subset \mathbb{C}$. If $f(z)$ is compact for z in an open set $S \subset R$, then $f(z)$ is compact for all $z \in R$.

Proof Suppose that $f(z_0)$ is not compact. Since the compact operators are closed, we can find, by the Hahn–Banach theorem, a linear functional $L \in \mathscr{L}(\mathscr{H})^*$ so that $L(f(z_0)) = 1$ and $L(A) = 0$ if A is compact. Then $L(f(z))$ is analytic, $L(f(z)) = 0$ if $z \in S$ and $L(f(z_0)) = 1$. Since S is open, this is impossible. We conclude that $f(z_0)$ is compact for all z_0. ∎

This last lemma can also be proven using the idea of analytic continuation by power series.

Proof of Theorem XIII.17 in case $N = 3$, $V_{ij} \in L^2$ Since $I(E)$ is a compact operator-valued function on $\mathbb{C}\backslash[\Sigma, \infty)$ and $1 - I(E)$ is invertible if E is real and very negative, the analytic Fredholm theorem (Theorem VI.14) implies that there is a discrete set $S \subset \mathbb{C}\backslash[\Sigma, \infty)$ so that $(1 - I(E))^{-1}$ exists and is analytic in $\mathbb{C}\backslash([\Sigma, \infty) \cup S)$ and is meromorphic in $\mathbb{C}\backslash[\Sigma, \infty)$ with finite rank residues. Thus $[1 - I(E)]^{-1}D(E) \equiv f(E)$ is analytic in $\mathbb{C}\backslash([\Sigma, \infty) \cup S)$ with finite rank residues at points of S. Let $E \notin S$, $\operatorname{Im} E \neq 0$. Then, by (24),

$f(E) = (H - E)^{-1}$. In particular, $f(E)(H - E)\psi = \psi$ for any $\psi \in D(H)$. By analytic continuation, this holds for any $E \notin S \cup [\Sigma, \infty)$. We conclude that, for any such E, $H - E$ has a bounded inverse. Thus any point of $\sigma(H) \backslash [\Sigma, \infty)$ must be in S, so $\sigma(H) \backslash [\Sigma, \infty)$ consists of isolated points with only Σ as a possible limit point. Finally, since $(H - E)^{-1}$ has finite rank residues at any point $\lambda \in S$, we conclude that the spectral projection

$$P_\lambda = (-2\pi i)^{-1} \oint_{|E-\lambda|=\varepsilon} (H - E)^{-1}\, dE$$

is finite dimensional, i.e., any $\lambda \in \sigma(H) \backslash [\Sigma, \infty)$ is in $\sigma_{\text{disc}}(H)$. ∎

The proof in the general case involves no additional analytic ideas but we need to overcome two complications: (1) V_{ij} need only be in $R + (L^\infty)_\varepsilon$; (2) the diagrammatic analysis is not so simple if $N > 3$ and it is necessary to develop some combinatorial machinery. Since V_{ij} is, in general, only form bounded, we must deal with expressions like $(H_0 - E)^{-1/2} V_{ij} (H_0 - E)^{-1/2}$ rather than $V_{ij}(H_0 - E)^{-1}$. We therefore revise our graphical rules: Given a diagram with successive pairwise links of n horizontal lines, associate a factor of $-G_0^{1/2}(E) V_{ij} G_0^{1/2}(E)$ with each link between i and j and no additional factors corresponding to the horizontal lines. This changes the operator that we associated to a diagram before by removing a factor of $G_0^{1/2}$ from each end. By $G_0^{1/2}$ we mean the operator that acts in momentum space as multiplication by $(p^2 - E)^{-1/2}$ where we take the square root branch that is positive if $E < 0$. We shall consider the case of general $N \geq 3$, and (21) will henceforth denote the analogous general expansion for such N.

Lemma 3B Let $V_{ij} \in R + (L^\infty)_\varepsilon$. Let G be a diagram in the formal expansion (21). Then the operator associated with G according to the graphical rules *just discussed* is compact if and only if G is connected.

Proof As before, if the diagram is disconnected, it is noncompact, so suppose that G is a fixed connected diagram. Let $V_{ij} \in \mathscr{S}(\mathbb{R}^3)$ for each ij. We shall first show that under such circumstances (actually $V_{ij} \in L^2$ suffices) the associated operator G is Hilbert–Schmidt and thus compact.

The proof will be by induction on N, the number of lines in the graph. For $N = 1$, the Hilbert space is $\mathbb{C}$ so the operator (which is 1) is certainly Hilbert–Schmidt. Thus, we suppose that all connected graphs with fewer than N lines are known to be Hilbert–Schmidt.

We first note that we may as well suppose that G is barely connected since any G can be written as $G = G_1 G_2$ with G_2 bounded and G_1 barely connected. By relabeling lines we can suppose that the last link in G connects

lines i and $i+1$ and that if this last line is removed, then the graph remaining has two connected pieces, one containing lines $1, \ldots, i$; the other $i+1, \ldots, N$.

Pick new coordinates $R_1, \ldots, R_{N-1}$ by $R_j = r_{j+1} - r_j$ and let $P_1, \ldots, P_{N-1}$ be the corresponding momentum operators, i.e., P_j is $-i\nabla_{R_j}$, the partial derivative being taken with $R_1, \ldots, R_{j-1}, R_{j+1}, \ldots, R_{N-1}$ fixed. Let W_{jk} be the function given by $\hat{W}_{jk} = |\hat{V}_{jk}|$ and define the operator $A(jk)$ as

$$A(jk) = \begin{cases} \left(\sum_{\ell \le i-1} P_\ell^2 + 1\right)^{-1/2} W_{jk} \left(\sum_{\ell \le i-1} P_\ell^2 + 1\right)^{-1/2} & \text{if} \quad j,k \le i \\ (P_i^2+1)^{-1/2} W_{i,i+1} (P_i^2+1)^{-1/2} & \text{if} \quad j=i,\ k=i+1 \\ \left(\sum_{\ell \ge i+1} P_\ell^2 + 1\right)^{-1/2} W_{jk} \left(\sum_{\ell \ge i+1} P_\ell^2 + 1\right)^{-1/2} & \text{if} \quad j,k \ge i+1 \end{cases}$$

Let $\tilde{G}$ be the operator obtained by replacing each factor $G_0^{1/2}(E)V_{jk}\,G_0^{1/2}(E)$ in G by $A(jk)$. We first claim that $\tilde{G}$ is Hilbert–Schmidt: For under the decomposition

$$L^2(\mathbb{R}^{3N-3}) = L^2(\mathbb{R}^{3i-3}) \otimes L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^{3N-3i-3})$$

corresponding to $\langle R_1, \ldots, R_{i-1}\rangle$, R_i, $\langle R_{i+1}, \ldots, R_{N-1}\rangle$, $\tilde{G}$ is a tensor product $A \otimes B \otimes C$ where A and C are operators associated to graphs with i and $N-i$ lines respectively. B is explicitly seen to be Hilbert–Schmidt on $L^2(\mathbb{R}^3)$, for example by writing its kernel in p space (i.e., looking at $\mathscr{F}B\mathscr{F}^{-1}$) and A and C are, by the induction hypothesis, Hilbert–Schmidt on $L^2(\mathbb{R}^{3i-3})$ and $L^2(\mathbb{R}^{3N-3i-3})$, respectively. Thus $\tilde{G}$ is Hilbert–Schmidt.

Now let $g = \mathscr{F}G\mathscr{F}^{-1}$ and $\tilde{g} = \mathscr{F}\tilde{G}\mathscr{F}^{-1}$. Since $|\hat{V}_{ij}| \le \hat{W}_{ij}$ and $|H_0 - E| \ge c_0(\sum_{\ell=1}^{N+1} P_\ell^2 + 1)$ for some constant c_0, the kernel of g is majorized by a multiple of the kernel of $\tilde{g}$. Since $\tilde{g}$ is Hilbert–Schmidt, so is g and thus so is G.

Now suppose that $V_{ij} \in R + (L^\infty)_\varepsilon$. We can find $V_{ij}^{(n)} \in \mathscr{S}(\mathbb{R}^3)$ so that $\|(H_0 - E)^{-1/2}(V_{ij} - V_{ij}^{(n)})(H_0 - E)^{-1/2}\| \to 0$ as $n \to \infty$ (Problem 44). Given any connected diagram G, let $g^{(n)}$ be the associated operator if potentials $V_{ij}^{(n)}$ are used and let g be the associated operator if V_{ij} is used. Then $g^{(n)} \to g$ in norm. Since each $g^{(n)}$ is compact, g is compact. ∎

We now turn to the combinatorics necessary to find closed expressions for $D_R(E)$, the sum of all disconnected diagrams, and $I_R(E)$, the sum of all barely connected diagrams.

Definition Let G be a diagram with N labeled horizontal lines and some vertical links of pairs. G is called k-**connected** if it has k connected components. The **cluster decomposition** $D(G)$ associated with G is the family of sets of lines linked to one another.

Thus, the diagram in Figure XIII.3 is 2-connected with $D(G) = \{\{1, 2, 4\}, \{3, 5\}\}$.

Definition The **associated string** of a k-connected diagram is a set of cluster decompositions $D_N, \ldots, D_k$ defined as follows. Suppose G has ℓ links. Let $G_0, \ldots, G_\ell$ be the diagrams obtained by keeping the first $0, 1, \ldots, \ell$ links (counting from the left). Consider the cluster decompositions $D(G_0), \ldots, D(G_\ell)$. D_m is the $(N + 1 - m)$th *distinct* decomposition in the family $D(G_0), \ldots, D(G_\ell)$. It has exactly m clusters. We write $S(G)$ for the associated string of G.

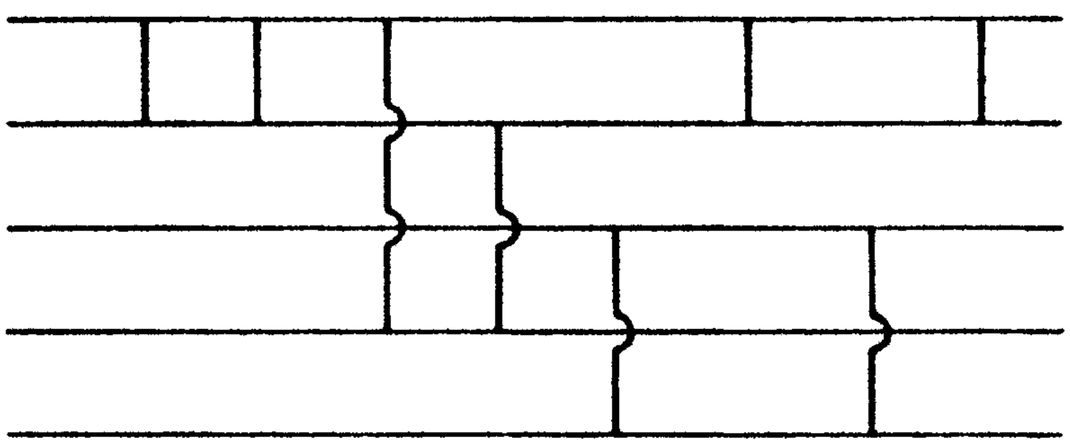


FIGURE XIII.3 A 2-connected diagram.

Thus, the diagram in Figure XIII.3 has

$$D_5 = \{\{1\}, \{2\}, \{3\}, \{4\}, \{5\}\}$$

$$D_4 = \{\{1, 2\}, \{3\}, \{4\}, \{5\}\}$$

$$D_3 = \{\{1, 2, 4\}, \{3\}, \{5\}\}$$

$$D_2 = \{\{1, 2, 4\}, \{3, 5\}\} \equiv D(G)$$

Notice that $D_5 = D(G_0)$; $D_4 = D(G_1) = D(G_2)$; $D_3 = D(G_3) = D(G_4)$; $D_2 = D(G_5) = D(G_6) = D(G_7) = D(G_8)$.

Finally, we define:

Definition A **string** S is a family $D_N, D_{N-1}, \ldots, D_k$ of cluster decompositions of $\{1, \ldots, N\}$ so that $D_{j+1} \rhd D_j$ and so that D_j has j clusters. The string is called connected if $k = 1$ and **disconnected** if $k > 1$. k will be called the **index** of S and we write $i(S) = k$.

We recall from Section XI.5 that $D \rhd D'$ means that each cluster in D' is a union of clusters in D. Thus, if S is a string, D_j is obtained from D_{j+1} by lumping one pair of clusters together. Also, iDm means that i and m are indices in the same cluster of D and $\sim iDm$ means that they are in different clusters.

To sum up all disconnected diagrams, we shall first sum all diagrams with the same associated string and then sum over the (finitely many) strings. In the following, the symbols

$$\sum_{D} \quad \text{and} \quad \sum_{D \sim D'}$$

stand respectively for the sum over those pairs ij with $i < j$ and iDj (respectively iDj and not $iD'j$).

Definition Let $S_0 = \langle D_N, D_{N-1}, \ldots, D_k \rangle$ be a fixed string and let E be so negative that

$$\sum_{1 \le i < j \le N} \| (H_0 - E)^{-1/2} V_{ij} (H_0 - E)^{-1/2} \| < 1 \tag{25}$$

Given any cluster decomposition D, we define the **reduced resolvent** $R_D(E)$ by

$$R_D(E) = \left[1 + (H_0 - E)^{-1/2} \left(\sum_{D} V_{ij} \right) (H_0 - E)^{-1/2} \right]^{-1} \tag{26}$$

Define $I_{D_m D_{m-1}}$ by

$$I_{D_m D_{m-1}} = (H_0 - E)^{-1/2} \left(- \sum_{D_{m-1} \sim D_m} V_{ij} \right) (H_0 - E)^{-1/2} \tag{27}$$

Finally, let $R_{S_0}(E)$ be the convergent sum of all diagrams G with $S(G) = S_0$. The sum (27) can be described as follows. D_{m-1} differs from D_m by having two clusters C_ℓ and C_p in D_m being replaced in D_{m-1} by the single cluster $C_q = C_p \cup C_\ell$. The sum in (27) is over those $i < j$ with $i \in C_\ell$, $j \in C_p$ or $i \in C_p$, $j \in C_\ell$.

Lemma 6

$$R_{S_0}(E) = R_{D_N}(E) I_{D_N D_{N-1}} R_{D_{N-1}}(E) I_{D_{N-1} D_{N-2}} \cdots I_{D_{k+1}} I_{D_k} R_{D_k}(E) \tag{28}$$

Proof Any arbitrary diagram G with $S(G) = S_0$ can be described as follows. The first link must change the cluster decomposition from D_N to D_{N-1} and so must be of the form $-(H_0 - E)^{-1/2} V_{ij} (H_0 - E)^{-1/2}$ with $\sim iD_N j$ and $iD_{N-1} j$. Then there are an arbitrary number of links that do not change the associated clustering. These must be i, j links with $iD_{N-1} j$. Next follows a

link that changes the clustering from D_{N-1} to D_{N-2}, etc. If we write $W_{ij} = -(H_0 - E)^{-1/2} V_{ij} (H_0 - E)^{-1/2}$, we see that

$$R_{S_0}(E) = \left(\sum_{D_{N-1} \sim D_N} W_{ij} \right) \left(\sum_{\ell=0}^{\infty} \left(\sum_{D_{N-1}} W_{ij} \right)^{\ell} \right) \left(\sum_{D_{N-2} \sim D_{N-1}} W_{ij} \right) \cdots$$

Since $\sum_{i<j} \| W_{ij} \| < 1$, all the infinite sums converge and (28) results. ∎

Let $\mathscr{H}_{+1}$, $\mathscr{H}_{-1}$ be the scale of spaces associated with H_0 (see Section VIII.6). Let D be a cluster decomposition with $\#(D) \geq 2$ and suppose that $E \in \mathbb{C} \backslash [\Sigma, \infty)$. Then $E \notin \sigma(H_D)$. By the construction of sums of quadratic forms, $(H_D - E)^{-1}$ maps $\mathscr{H}_{-1}$ boundedly onto $\mathscr{H}_{+1}$, so

$$\begin{aligned} &(H_0 - E)^{+1/2} (H_D - E)^{-1} (H_0 - E)^{+1/2} \\ &\quad = [1 + (H_0 - E)^{-1/2} \sum_D V_{ij} (H_0 - E)^{-1/2}]^{-1} \end{aligned}$$

defines a bounded operator, which we denote by $R_D(E)$ consistently with the definition (26). For $E \notin [\Sigma, \infty)$, we *define* $R_{S_0}(E)$ by (28) whenever S_0 is a string with $i(S_0) \geq 2$. Lemma 6 shows that when E is very negative this definition is consistent with the definition as the sum of all graphs with string S_0. We are now ready to define the objects required for a general Weinberg–Van Winter equation. The symbol $\sum_{S,\, i(S)=2}$ means the sum over all strings of index 2.

Definition The **reduced disconnected part** is defined for $E \notin [\Sigma, \infty)$ by

$$D_R(E) = \sum_{S,\, i(S) \geq 2} R_S(E) \tag{29a}$$

The **symmetrized Weinberg kernel** is defined by

$$I_R(E) = - \sum_{S,\, i(S)=2} R_S(E) \left[\sum_{\sim D_2} (H_0 - E)^{-1/2} V_{ij} (H_0 - E)^{-1/2} \right] \tag{29b}$$

In (29b), D_2 refers to the last decomposition in the string S involved in the particular summand. Note that in (29) the sum over strings is a *finite* sum.

Lemma 4B $D_R(E)$ and $I_R(E)$ are analytic in $\mathbb{C} \backslash [\Sigma, \infty)$ and $I_R(E)$ is compact operator valued with $\lim_{E \to -\infty} \| I_R(E) \| = 0$. For $E \notin \sigma(H)$, let

$$R(E) \equiv R_{\{(1, \ldots, N)\}}(E) = \left[1 + (H_0 - E)^{-1/2} \left(\sum_{i<j} V_{ij} \right) (H_0 - E)^{-1/2} \right]^{-1}$$

where $\{\{1, \ldots, N\}\}$ refers to the cluster decomposition D with one cluster. Then for all $E \notin \sigma(H)$,

$$R(E) = D_R(E) + I_R(E)R(E) \tag{29c}$$

Proof Any D with $\#(D) \geq 2$ has $\sigma(H_D) \subset [\Sigma, \infty)$ so $I_R(E)$ and $D_R(E)$ are analytic in $\mathbb{C}\backslash[\Sigma, \infty)$. For all E with sufficiently negative real part, $I_R(E)$ can be expanded into the norm convergent sum of all barely connected diagrams. By Lemma 3B, $I_R(E)$ is compact for all such E, so, by Lemma 5, $I_R(E)$ is compact for all $E \in \mathbb{C}\backslash[\Sigma, \infty)$. From the perturbation series, it also follows that $\lim_{E \to -\infty} \|I_R(E)\| = 0$.

Next notice that there is a one–one correspondence between strings S with $i(S) = 2$ and strings $\tilde{S}$ with $i(\tilde{S}) = 1$ for the only decomposition with one element is $D_1 \equiv \{\{1, \ldots, N\}\}$ and that $R_{D_1} = R$. Thus if $S = \langle D_N, \ldots, D_2 \rangle$ and $\tilde{S} = \langle D_N, \ldots, D_1 \rangle$, Lemma 6 implies that

$$R_{\tilde{S}}(E) = -R_S(E)\left[\sum_{\sim D_2} (H_0 - E)^{-1/2} V_{ij} (H_0 - E)^{-1/2}\right] R(E)$$

Summing over all $\tilde{S}$ (equivalently all S), we see that

$$\sum_{\tilde{S},\, i(\tilde{S})=1} R_{\tilde{S}}(E) = I_R(E)R(E)$$

For all sufficiently negative E, the perturbation series (21) converges so $R(E)$ is the sum over all diagrams; and thus summing first over diagrams in each fixed string and then over strings, we conclude that

$$R(E) = \sum_{S,\, i(S) \geq 2} R_S(E) + \sum_{\tilde{S},\, i(\tilde{S})=1} R_{\tilde{S}}(E)$$

This proves (29c) when E is very negative. By analytic continuation it holds for $E \notin \sigma(H) \cup [\Sigma, \infty) = \sigma(H)$ (by Lemma 2). ∎

(29) is called the **Weinberg–Van Winter equation.**

Proof of Theorem XIII.17, general case The proof is essentially the same as in the special case $N = 3$; $V_{ij} \in L^2$. By Lemma 4B and the analytic Fredholm theorem, $(I - I_R(E))^{-1}$ exists and is analytic in $\mathbb{C}\backslash([\Sigma, \infty) \cup S)$ where S is a discrete set in $\mathbb{C}\backslash[\Sigma, \infty)$. Thus

$$f(E) = (H_0 - E)^{-1/2}[1 - I_R(E)]^{-1} D_R(E)(H_0 - E)^{-1/2}$$

exists in $\mathbb{C}\backslash([\Sigma, \infty) \cup S)$ with finite rank residues at points of S. When $\operatorname{Im} E \neq 0$, $f(E) = (H - E)^{-1}$ so for all $\psi \in D(H)$, $f(E)(H - E)\psi = \psi$. By analytic continuation $\sigma(H) \subset [\Sigma, \infty) \cup S$ and the points of S have finite spectral projections. Thus $\sigma_{\text{ess}}(H) \subset [\Sigma, \infty)$. By Lemma 2, $[\Sigma, \infty) \subset \sigma(H)$ so $\sigma_{\text{ess}}(H) = [\Sigma, \infty)$. ∎

As an immediate corollary of the HVZ theorem, we have

Theorem XIII.18 If H is an N-body Schrödinger operator with center of mass removed and if $V_{ij} \in L^2 + L^r$ $(r < 3)$ for all i, j, then $\sigma_{ac}(H) = [\Sigma, \infty)$ with Σ given by (20b).

Proof From Theorem XI.34, and the relations

$$e^{-iHt}\Omega_D^{\pm} = \Omega_D^{\pm} e^{-iH_D t} \qquad \text{and} \qquad (\Omega_D^{+})^* \Omega_D^{+} = 1$$

it follows that $\sigma_{ac}(H) \supset \sigma_{ac}(H_D)$ for all D. If $\#(D) \geq 2$, then $\sigma_{ac}(H_D) = \sigma(H_D) = [\Sigma_D, \infty)$ so $\sigma_{ac}(H) \supset [\Sigma, \infty)$. On the other hand, $\sigma_{ac}(H) \subset \sigma_{ess}(H) = [\Sigma, \infty)$ by the HVZ theorem. ∎

We want to conclude this section by giving a second proof of the "hard" part of Theorem XIII.17, i.e., that $\sigma_{ess}(H) \subset [\Sigma, \infty)$. This proof uses very different ideas but is also based on a compactness condition, namely:

Lemma 7 Let H be a self-adjoint operator so that $f(H)$ is compact for every continuous function f of compact support with $\operatorname{supp} f \subset (-\infty, \Sigma)$. Then $\sigma_{ess}(H) \subset [\Sigma, \infty)$.

Proof This is a part of Theorem XIII.77 which is proven in Section 14. ∎

Our second proof that $\sigma_{ess}(H) \subset [\Sigma, \infty)$ is based on two ideas. First, bounded regions cannot contribute to $\sigma_{ess}(H)$ and, secondly, near infinity, H must look like some H_D. To express the first idea, we pick a function $\varphi \in C_0^{\infty}(\mathbb{R}^{3N-3})$ with $0 \leq \varphi \leq 1$, so that $\varphi(x) = 1$ if $|x| \leq 1$ and $\varphi(x) = 0$ if $|x| \geq 2$. Define $j_{\leq n}(x) = \varphi(xn^{-1})$ and $j_{\geq n} = 1 - j_{\leq n}$. The first idea is expressed by:

Lemma 8 Let H obey the hypotheses of Theorem XIII.17. Then for each continuous function f of compact support and for each n, $j_{\leq n} f(H)$ is compact.

Proof Pick $C < \inf \sigma(H)$ and a bounded continuous function g so that $g(x) = (x - c)^{1/2} f(x)$ for $x \in \sigma(H)$. Then

$$j_{\leq n} f(H) = j_{\leq n}(H - c)^{-1/2} g(H) =$$
$$j_{\leq n}(H_0 + 1)^{-1/2}[(H_0 + 1)^{1/2}(H - c)^{-1/2}]g(H)$$

Thus it suffices to prove that $j_{\leq n}(H_0 + 1)^{-1/2}$ is compact. This follows from Theorem XI.20 or Problem 41. ∎

To express the notion that H looks like some H_D near infinity, at least in suitable tubes, the following is useful:

Lemma 9 Let A_n be a family of bounded operators with $\sup_n \|A_n\| < \infty$ and let H_1, H_2 be two self-adjoint operators with $\sigma(H_1)$ and $\sigma(H_2)$ contained in $[c, \infty)$ so that

$$\lim_{n\to\infty} \|A_n[(H_1 - z)^{-1} - (H_2 - z)^{-1}]\| = 0$$

for all z in some open subset of $\mathbb{C}\backslash[c, \infty)$. Then

$$\lim_{n\to\infty} \|A_n[f(H_1) - f(H_2)]\| = 0$$

for any continuous function f of compact support.

Proof The proof is similar to that of Theorem VIII.20a. By the Vitali convergence theorem, the first limiting statement holds for all z in $\mathbb{C}\backslash[c, \infty)$ and uniformly on compact subsets of $\mathbb{C}\backslash[c, \infty)$. Using the Cauchy integral formula, we conclude that

$$\lim_{n\to\infty} \|A_n[(H_1 - c + 1)^{-m} - (H_2 - c + 1)^{-m}]\| = 0$$

The lemma now follows from the Stone–Weierstrass theorem which implies that $f(x)$ can be uniformly approximated on $[c, \infty)$ by polynomials in $(x - c + 1)^{-1}$. ∎

Next we single out the regions in which H and H_D look alike. Only D's with $\#(D) = 2$ will be needed, so let D_a, $a = 1, 2, \ldots, 2^{N-1} - 1$ label all the distinct ways of decomposing $\{1, \ldots, N\}$ into two nonempty sets $C_a^{(1)}$ and $C_a^{(2)}$. Define, $H_a = H_{D_a}$, $I_a = I_{D_a}$, and

$$|x|_0 = \left(\sum_{i\le j} |x_i - x_j|^2\right)^{1/2}$$

$$|x|_a = \min\{|x_i - x_j| \mid i \in C_a^{(1)}, j \in C_a^{(2)}\}$$

Lemma 10 Let $d_N = (N-1)^{-3/2}N^{-1/2}\sqrt{2}$. Then for any $x \in \mathbb{R}^{3N-3}$, there is an a so that $|x|_a \ge d_N |x|_0$. In particular, there exist functions j_a, $a = 1, \ldots, 2^{N-1} - 1$ so that

(a) $0 \le j_a \le 1$, $\sum_a j_a(x) \equiv 1$.

(b) $j_a(\lambda x) = j_a(x)$, all $\lambda \in (0, \infty)$.

(c) j_a is C^∞ on $\mathbb{R}^{3N-3}\backslash\{0\}$.

(d) Supp $j_a \subset \{x \mid |x|_a \ge \frac{1}{2}d_N|x_0|\}$.

Proof This is a geometric proof identical to one given in our discussion of the Haag-Ruelle scattering theory (Section XI.16). Given x, let i and j be two points with $|x_i - x_j| \geq \sqrt{2}N^{-\frac{1}{2}}(N-1)^{-\frac{1}{2}}|x|_0$. Let $\pi_1, \ldots, \pi_N$ be the N planes through $x_1, \ldots, x_N$ perpendicular to $x_i - x_j$. Clearly they divide the region between π_i and π_j into at most $(N-1)$ slabs one of which must have thickness at least $(N-1)^{-1}|x_i - x_j|$. Choosing $C_a^{(1)}$ and $C_a^{(2)}$ to be the particles on each side of this slab, we have $|x|_a \geq (N-1)^{-1}|x_i - x_j|$.

To construct the j_a's, we first consider the open subsets of the sphere $S \equiv \{x \,|\, |x|_0 = 1\}$ of the form $R_a = \{x \,|\, |x|_a \geq \frac{1}{2}d_N, |x|_0 = 1\}$ which by the above cover S. In the usual way, we find C^∞ functions $\tilde{j}_a$ on S with $\operatorname{supp} \tilde{j}_a \subset R_a$, $0 \leq \tilde{j}_a$ and $\sum \tilde{j}_a \equiv 1$. We take $j_a(x) = \tilde{j}_a(|x|_0^{-1}x)$. ∎

We can now give a precise meaning to the fact that "near infinity" H looks like some H_a.

Lemma 11 Fix $a = 1, \ldots, 2^{N-1} - 1$. For any $z \notin \sigma(H) \cup \sigma(H_a)$,

$$\lim_{n \to \infty} \|j_{\geq n} j_a[(H-z)^{-1} - (H_a - z)^{-1}]\| = 0$$

Proof Writing

$$j_{\geq n} j_a[(H-z)^{-1} - (H_a - z)^{-1}] \equiv -(H-z)^{-1} I_a j_a j_{\geq n}(H_a - z)^{-1} + [(H-z)^{-1}, j_{\geq n} j_a] I_a (H_a - z)^{-1}$$

and using $[(H-z)^{-1}, f] = -(H-z)^{-1}[H_0, f](H-z)^{-1}$, we see that it suffices to prove that

$$\|(H_0 + 1)^{-1/2} I_a j_a j_{\geq n}(H_0 + 1)^{-1/2}\| \to 0 \tag{29.1}$$

and

$$\|(H_0 + 1)^{-1/2}[H_0, j_{\geq n} j_a](H_0 + 1)^{-1/2}\| \to 0 \tag{29.2}$$

Since $j_a j_{\geq n}$ is supported in the region where $|x|_a \geq \frac{1}{2}d_N n$, (29.1) follows from the fact that V_{ij} is in $R + L_\varepsilon^\infty$. (29.2) follows from the fact that

$$\|\nabla(j_{\geq n} j_a)\|_\infty \leq \|j_{\geq n} \nabla j_a\|_\infty + \|\nabla j_{\geq n}\|_\infty = Cn^{-1} \to 0$$ ∎

Second proof of Theorem XIII.17 We give a second proof that $\sigma_{\text{ess}}(H) \subset [\Sigma, \infty)$. Since $\sum j_a = j_{\leq n} + j_{\geq n} = 1$, we have

$$f(H) = f(H) j_{\leq n} + \sum_a [f(H) - f(H_a)] j_a j_{\geq n} + \sum_a f(H_a) j_a j_{\geq n} \tag{29.3}$$

Let f be a continuous function of compact support with $\operatorname{supp} f \subset (-\infty, \Sigma]$. Since $\sigma(H_a) \subset [\Sigma, \infty)$, we have that $f(H_a) = 0$, so the last term in (29.3) is zero. By Lemmas 9 and 11, the second term in (29.3) goes to zero in norm

as $n \to \infty$. By Lemma 8, the first term is compact. Thus, for such f's, $f(H)$ is compact. By Lemma 7, we conclude that $\sigma_{ess}(H) \subset [\Sigma, \infty)$. ∎

Finally, we note that (29.3) is useful for considering the case where we restrict to suitable symmetry subspaces. The abstract theorem is

Theorem XIII.17′ Let H be an operator obeying the hypotheses of Theorem XIII.17. Let P be the projection onto an invariant subspace for H and P_a, $a = 1, \ldots, 2^{N-1} - 1$ the projections onto some invariant subspace for H_a containing $P\mathscr{H}$. Let $\Sigma_P = \min_a \inf \sigma(H_a P_a)$. Then $\sigma_{ess}(HP) \subset [\Sigma_P, \infty)$.

Proof Clearly $\Sigma_P \leq 0$ since $0 \in \sigma(H_a P_a)$. Thus, for any f supported in $(-\infty, \Sigma_P)$, $Pf(H) = f(PH)$ and $P_a f(H_a) = f(P_a H_a) = 0$. Since $P = PP_a$, by hypothesis, we have that

$$f(PH) = Pf(H)j_{\leq n} + P \sum_a [f(H) - f(H_a)]j_a j_{\geq n}$$

on account of (29.3). As in the above proof, we conclude that $f(PH)$ is compact and thus that $\sigma_{ess}(HP) \subset [\Sigma_P, \infty)$. ∎

Example Consider H, the Hamiltonian of an atom, that is, the operator obtained by removing the center of mass from

$$\tilde{H} = -\sum_{i=1}^{N-1} (2\mu)^{-1} \Delta_i - (2M)^{-1} \Delta_N - Z \sum_{i=1}^{N-1} |r_i - r_N|^{-1} + \sum_{i<j\leq N-1} |r_i - r_j|^{-1}$$

and let P be the projection onto all functions antisymmetric under interchange of the r_i's, $i = 1, \ldots, N-1$. For each a, let P_a be the projection onto all functions antisymmetric under interchange of two electrons in the same $C_j^{(a)}$. Then, Theorem XIII.17′ implies that $\sigma_{ess}(HP) \subset [\Sigma_P, \infty)$ which is generally strictly smaller than $[\Sigma, \infty)$. One can show easily (Problem 46) that $[\Sigma_P, \infty) \subset \sigma_{ess}(HP)$ in this case.

XIII.6 The absence of singular continuous spectrum I: General theory

Spectral analysis of an operator A concentrates on identifying the five sets $\sigma_{ess}(A)$, $\sigma_{disc}(A)$, $\sigma_{ac}(A)$, $\sigma_{sing}(A)$, $\sigma_{pp}(A)$. For large classes of Schrödinger operators H, we have succeeded in identifying $\sigma_{ess}(H)$ and $\sigma_{ac}(H)$. A precise determination of $\sigma_{disc}(H)$ is a detailed question, but we have seen how to use

the min–max principle to obtain a lot of information about it. That leaves $\sigma_{\text{sing}}(H)$ and $\sigma_{\text{pp}}(H)$. We shall discuss the question of proving $\sigma_{\text{pp}} = \sigma_{\text{disc}}$ in Section 13. The next five sections involve the difficult study of $\sigma_{\text{sing}}(H)$. Our discussion of asymptotic completeness in Section XI.3 suggests that $\sigma_{\text{sing}}(H) = \varnothing$ and our main goal will be the proof of this fact for various classes of Schrödinger operators.

As we have already emphasized, there are close connections between proving the absence of singular continuous spectrum and scattering theory. In fact, the development of eigenfunction expansions in Section XI.6 already tells us something about the singular spectrum. In general when $V \in L^1 \cap R$ we know that $\sigma_{\text{sing}} \subset \mathscr{E}$, the exceptional set, so that σ_{sing} has Lebesgue measure 0. And in two cases, first when $V \in L^1 \cap R$ and $\|V\|_R < 4\pi$, and secondly, if $Ve^{a|x|} \in R$ for some $a > 0$, we know that $\mathscr{E}$ is discrete so that $\sigma_{\text{sing}} = \varnothing$. In this section we shall develop a fundamental criterion for the absence of singular spectrum and show how it allows us to recover these two results from first principles without very much effort. In Sections 7 and 8, we shall use the connection between scattering theory and spectral analysis in reverse: The techniques developed to prove that there is no singular continuous spectrum will yield very strong results on asymptotic completeness.

The fundamental criterion for the absence of singular spectrum is very simple. In part it will depend on Stone's formula (Theorem VII.13):

$$\tfrac{1}{2}(\varphi, (E_{[a,b]} + E_{(a,b)})\varphi) = \lim_{\varepsilon \downarrow 0} \pi^{-1} \int_a^b \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx$$

where $R(\lambda)$ is the resolvent $(H - \lambda)^{-1}$ of some self-adjoint H and $\{E_\Omega\}$ is its family of spectral projections. In particular, one has that

$$\sup_{0<\varepsilon<1} \int_a^b |\operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)|^p\, dx < \infty \tag{30}$$

in the case $p = 1$ for any $\varphi \in \mathscr{H}$.

Theorem XIII.19 Let H be a self-adjoint operator with resolvent $R(\lambda) = (H - \lambda)^{-1}$. Let (a, b) be a bounded interval and $\varphi \in \mathscr{H}$. Suppose that there is a $p > 1$ for which (30) holds. Then $E_{(a,b)}\varphi \in \mathscr{H}_{ac}$.

Proof By Stone's formula and the fact that $E_{(c,d)} \leq E_{[c,d]}$

$$(\varphi, E_{(c,d)}\varphi) \leq \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \int_c^d \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx$$

for each open interval (c, d). Let S be an open set in (a, b) so that $S = \bigcup_{i=1}^{N} (a_i, b_i)$ is a union of disjoint open intervals. Suppose first that $N < \infty$. Then

$$(\varphi, E_S\varphi) \leq \frac{1}{\pi} \sum_{i=1}^{N} \lim_{\varepsilon \downarrow 0} \int_{a_i}^{b_i} \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx$$

$$\leq \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \sum_{i=1}^{N} \int_{a_i}^{b_i} \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx$$

$$\leq \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \left[\int_{a}^{b} |\operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)|^p\, dx \right]^{1/p} |S|^{1/q}$$

$$\leq C\,|S|^{1/q}$$

where $|S|$ is the Lebesgue measure of S and q is the conjugate index to p. If N is infinite, let $S_m = \bigcup_{i=1}^{m} (a_i, b_i)$. Then

$$(\varphi, E_S\varphi) = \lim_{m \to \infty} (\varphi, E_{S_m}\varphi) \leq \lim_{m \to \infty} C\,|S_m|^{1/q} = C\,|S|^{1/q}$$

Let I be an arbitrary set of Lebesgue measure 0 inside (a, b). Since Lebesgue measure is outer-regular, we can find an open set $S^{(k)}$ with $I \subset S^{(k)}$ and $|S^{(k)}| < 1/k$. Thus

$$(\varphi, E_I\varphi) \leq \inf_k (\varphi, E_{S^{(k)}}\varphi) \leq C \inf_k |S^{(k)}|^{1/q} = 0$$

Thus the measure $\Omega \mapsto (\varphi, E_\Omega\varphi)$ is absolutely continuous on (a, b) so $E_{(a,b)}\varphi \in \mathscr{H}_{\text{ac}}$. ∎

Theorem XIII.20 Let H be a self-adjoint operator with resolvent $R(\lambda) = (H - \lambda)^{-1}$. Let (a, b) be a bounded interval. Suppose that there is a dense set D in $\mathscr{H}$ so that, for each $\varphi \in D$, (30) holds for some $p > 1$. Then H has purely absolutely continuous spectrum on (a, b), i.e., Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$. Conversely, if Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$, then there is a set D, dense in Ran $E_{(a,b)}$, so that (30) holds for any $p \geq 1$ including $p = \infty$ when $\varphi \in D$.

Proof The first half of the theorem follows from Theorem XIII.19. For the second half, let D be the set of vectors φ for which the spectral measure $d\mu_\varphi$ for H is of the form $f(x)\,dx$ where $f \in L^\infty$ with compact support in (a, b). By hypothesis, D is dense in Ran $E_{(a,b)}$. Moreover,

$$\operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi) = \int_{-\infty}^{\infty} g_\varepsilon(x - y) f(y)\, dy$$

where $g_\varepsilon(y) = \varepsilon(y^2 + \varepsilon^2)^{-1}$. Since $\|g_\varepsilon\|_1 = \pi$ independently of ε, (30) holds with $p = \infty$ by Young's inequality and thus for all p since (a, b) is finite. ∎

In most applications of Theorem XIII.20, one actually proves that $(\varphi, R(\lambda)\varphi)$ is bounded on $M = \{x + i\varepsilon \mid \varepsilon \in (0, 1), x \in (a, b)\}$ or more strongly that $(\varphi, R(\lambda)\varphi)$ has a continuous extension to $\bar{M}$. A typical application is:

Theorem XIII.21 Let $V \in R$, the Rollnik class, and let $H = -\Delta + V$ on $L^2(\mathbb{R}^3)$. Suppose that *either*:

(a) $\|V\|_R < 4\pi$;

or

(b) $Ve^{a|x|} \in R$ for some $a > 0$.

Then $\sigma_{\text{sing}}(H) = \varnothing$.

Proof (a) Since $\|V\|_R < 4\pi$, $|V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}$ has a Hilbert–Schmidt norm less than one uniformly for $\lambda \in \mathbb{C}\backslash[0, \infty)$ (see Section XI.6). Let $f \in C_0^\infty$ and note that $|f|^{1/2} \in R$. Then

$$\begin{aligned}|f|^{1/2}(H - \lambda)^{-1}|f|^{1/2} = {} & |f|^{1/2}(H_0 - \lambda)^{-1}|f|^{1/2} \\ & + \sum_{n=0}^{\infty}(-1)^{n+1}(|f|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}) \\ & \times (|V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2})^n \\ & \times (|V|^{1/2}(H_0 - \lambda)^{-1}|f|^{1/2})\end{aligned}$$

converges uniformly in Hilbert–Schmidt norm to an operator with norm less than $C_1 + C_2(1 - (4\pi)^{-1}\|V\|_R)^{-1}$. Thus

$$|(f, (H - \lambda)^{-1}f)| \leq \| |f|^{1/2}\|_2 \, \| |f|^{1/2}(H - \lambda)^{-1}|f|^{1/2}\|$$

is bounded on $\mathbb{C}\backslash[0, \infty)$. The fundamental criterion, Theorem XIII.19, thus implies that Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$ for *all* (a, b) so σ_{pp} and σ_{sing} are empty.

(b) As in our discussion in Section XI.6, $(1 + |V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2})^{-1}$ exists for all $\lambda \in \mathbb{C}\backslash[0, \infty)$ and has continuous boundary values as $\lambda \to x + i0$ as long as x avoids a finite set $\mathscr{E}$ of real numbers. Let $[a, b]$ be disjoint from $\mathscr{E}$. Then

$$\begin{aligned}|f|^{1/2}(H - \lambda)^{-1}|f|^{1/2} = {} & |f|^{1/2}(H_0 - \lambda)^{-1}|f|^{1/2} \\ & - (|f|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}) \\ & \times (1 + |V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2})^{-1}|V|^{1/2} \\ & \times (H_0 - \lambda)^{-1}|f|^{1/2}\end{aligned}$$

is a uniformly bounded operator on $\{x + i\varepsilon \mid 0 < \varepsilon < 1; x \in [a, b]\}$ whenever $f \in C_0^\infty$. As in (a), this implies that Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$ so $\sigma_{\text{sing}} \subset \mathscr{E}$, a finite set. This implies that $\sigma_{\text{sing}} = \varnothing$. ∎

Given the simple criterion, Theorem XIII.20, for $\sigma_{sing}(H)$ to be empty, one can reasonably ask why the problem of controlling the singular continuous spectrum is so much more difficult than that of identifying $\sigma_{ess}(H)$ (Sections 4 and 5) or $\sigma_{ac}(H)$ (Section XI.3). The reason is that σ_{sing} is much less stable under perturbations. To illustrate this, we describe the Aronszajn–Donoghue theory of the behavior of σ_{sing} under rank one perturbations. This theory should be compared with the Weyl theorem on invariance of σ_{ess} and the Kato–Birman theory of the invariance of σ_{ac}. Basic to the Aronszajn–Donoghue theory is the following combination of classical results of Fatou and de la Vallée Poussin:

Proposition Let ν be a finite Borel measure on $\mathbb{R}$ and let

$$F(z) = \int (x - z)^{-1}\, d\nu(x)$$

for $\operatorname{Im} z > 0$. Let $A_\nu = \{x \mid \lim_{\varepsilon \downarrow 0} F(x + i\varepsilon) = \infty\}$ and let

$$B_\nu = \{x \mid \lim_{\varepsilon \downarrow 0} F(x + i\varepsilon) = \Phi(x), \text{ a finite number with } \operatorname{Im} \Phi(x) \neq 0\}$$

Then $\nu(\mathbb{R} \setminus (A_\nu \cup B_\nu)) = 0$, $\nu \restriction A_\nu$ is singular relative to Lebesgue measure, and $\nu \restriction B_\nu$ is absolutely continuous.

Proofs of this result may be tracked down by consulting the reference in the notes. Now let H_0 be some self-adjoint operator on $\mathscr{H}$ and let $\varphi \in \mathscr{H}$ be a unit vector. Let P denote the projection onto φ and let

$$H_\alpha = H_0 + \alpha P$$

Let $\mathscr{H}'$ be the cyclic subspace for φ generated by H_0. Clearly all the H_α equal H_0 on $(\mathscr{H}')^\perp$ so we may as well suppose that $\mathscr{H}' = \mathscr{H}$, that is, we henceforth suppose that φ is cyclic for H_0. It follows that φ is also cyclic for H_α since

$$(H_\alpha - z)^{-1}\varphi = (H_0 - z)^{-1}\varphi - \alpha(\varphi, (H_0 - z)^{-1}\varphi)(H_\alpha - z)^{-1}\varphi$$

so that the span of $\{(H_\alpha - z)^{-1}\varphi\}$ is identical to the span of $\{(H_0 - z)^{-1}\varphi\}$. By this cyclicity result, H_α is unitarily equivalent to multiplication by x on $L^2(\mathbb{R}, d\nu_\alpha)$ for a suitable measure $d\nu_\alpha$.

Clearly,

$$F_\alpha(z) \equiv \int (x - z)^{-1}\, d\nu_\alpha(x) = (\varphi, (H_\alpha - z)^{-1}\varphi)$$

obeys

$$F_\alpha(z) = F_\beta(z) + (\beta - \alpha)F_\alpha(z)F_\beta(z)$$

on account of the resolvent equation

$$(H_\alpha - z)^{-1} = (H_\beta - z)^{-1} + (\beta - \alpha)(H_\alpha - z)^{-1} P (H_\beta - z)^{-1}$$

Thus, we have the basic equation:

$$F_\alpha(z) = F_\beta(z)(1 + (\alpha - \beta)F_\beta(z))^{-1} \tag{30.5}$$

Note that if $\lim_{\varepsilon \downarrow 0} F_\beta(z) = \infty$, then $\lim_{\varepsilon \downarrow 0} F_\alpha(z) = (\alpha - \beta)^{-1} \neq \infty$ for $\alpha \neq \beta$. Applying the proposition, we have proven the following striking *non-invariance* of σ_{sing}:

Theorem XIII.21.5 Let H_0 be a self-adjoint operator and let φ be a cyclic vector for H_0. Let

$$H_\alpha = H_0 + \alpha(\varphi, \cdot)\varphi$$

Then for $\alpha \neq \beta$ the singular (i.e., the union of pure point and singular continuous) parts of the spectral measures for H_α and H_β are mutually singular.

Example Let $d\nu_0 = dx \restriction [0, 1] + d\mu_C$, where $d\mu_C$ is the Cantor measure. Then $\sigma_{\text{ess}}(H_\alpha) = [0, 1]$ for all α on account of Weyl's theorem. Moreover, $F_0 = F_L + F_C$ in the obvious way, and

$$\lim_{\varepsilon \downarrow 0} \operatorname{Im} F_L(x + i\varepsilon) = \begin{cases} 1, & x \in (0, 1) \\ \frac{1}{2}, & x = 0, 1 \\ 0, & x \notin [0, 1] \end{cases}$$

Since $\operatorname{Im} F_C(z) \geq 0$ for all z with $\operatorname{Im} z > 0$, we see that $\lim_{\varepsilon \downarrow 0} F_0(x + i\varepsilon)$ is never real for any $x \in [0, 1]$. It follows from the basic equation (30.5) that $\lim_{\varepsilon \downarrow 0} F_\beta(x + i\varepsilon)$ is never infinite for $\beta \neq 0$, $x \in [0, 1]$. Thus, each H_β for $\beta \neq 0$ has no singular continuous spectrum while $\sigma_{\text{sing}}(H_0) \neq \varnothing$. Thus, we have two bounded operators H_0 and H_1 such that $H_0 - H_1$ has rank one, with $\sigma_{\text{sing}}(H_1) = \varnothing \neq \sigma_{\text{sing}}(H_0)$!

XIII.7 The absence of singular continuous spectrum II: Smooth perturbations

Theorem XIII.20 suggests that one study L^p bounds on expectation values of the resolvent and our experience suggests that $p = 2$ will be particularly easy to study.

Definition Let H be a self-adjoint operator with resolvent $R(\mu) = (H - \mu)^{-1}$. Let A be a closed operator. A is called **H-smooth** if and only if for each $\varphi \in \mathscr{H}$ and each $\varepsilon \neq 0$, $R(\lambda + i\varepsilon)\varphi \in D(A)$ for almost all $\lambda \in \mathbb{R}$ and moreover

$$\|A\|_H^2 = \sup_{\substack{\|\varphi\| = 1 \\ \varepsilon > 0}} \frac{1}{4\pi^2} \int_{-\infty}^{\infty} (\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2)\, d\lambda < \infty \quad (31)$$

Since A is closed, it is enough that (31) hold for a dense set of φ (Problem 47a). More interestingly, the uniform boundedness principle shows that if for *each* φ, $\int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2\, d\lambda \leq M_\varphi^2$ for a constant M_φ (independent of $\varepsilon > 0$ and of $\pm$, but dependent on φ), then A is H-smooth (Problem 47b,c).

The H-smooth operators are an especially nice class of operators. For example, we shall see that they are H-bounded with relative bound 0. They present in microcosm the close connection between scattering theory and spectral analysis. On one hand, we shall prove a basic result on the existence and completeness of wave operators $\Omega^{\pm}(H_1, H_0)$ when $H_1 - H_0$ is the product of an H_1-smooth operator and an H_0-smooth operator (Theorem XIII.24; see also Theorem XIII.31). On the other hand, we will see that if A is H-smooth, then $\overline{\text{Ran}(A^*)} \subset \mathscr{H}_{\text{ac}}(H)$ (Theorem XIII.23), which will lead to several theorems on the absence of singular continuous spectrum (see Theorems XIII.26 and XIII.28).

This section is divided into two parts. First, we shall develop the abstract theory of smooth perturbations, and in the second part we apply the theory to a variety of Schrödinger operators. The first two applications involve situations where the wave operators are unitary, i.e., where H and H_0 are unitarily equivalent. These are the cases of Schrödinger operators $H_0 + \lambda V$ with λ small or V repulsive. In the latter case, the theory of smooth perturbations will lead only to a proof that H has purely absolutely continuous spectrum. In our last application we shall establish the existence of wave operators for the case of repulsive potentials with some fall-off hypotheses by developing a generalization of the notion of H-smoothness. Part of this generalized theory will play a role in the next section.

One of our first main goals will be the reformulation of H-smoothness in a number of equivalent forms. We shall need the following vector-valued version of the Plancherel theorem.

Lemma 1 Let $\varphi(\cdot)$ be a (weakly measurable) function from $\mathbb{R}$ to a separable Hilbert space $\mathscr{H}$. Suppose that $\int \|\varphi(x)\|\, dx < \infty$. Define $\hat{\varphi}: \mathbb{R} \to \mathscr{H}$ by

$$\hat{\varphi}(p) = (2\pi)^{-1/2} \int_{\mathbb{R}} e^{-ipx}\varphi(x)\, dx$$

(where, by our standard convention, the integral is a weak integral). Let A be a closed operator on $\mathscr{H}$. Then

$$\int \|A\hat{\varphi}(p)\|^2 \, dp = \int \|A\varphi(x)\|^2 \, dx \tag{32}$$

where the integrals in (32) are set equal to ∞ if $\hat{\varphi}(p)$ (respectively, $\varphi(x)$) is not in $D(A)$ almost everywhere.

Proof First suppose that A is bounded. Then for any $\psi \in \mathscr{H}$, $(\psi, A\hat{\varphi}(p)) = (A^*\psi, \hat{\varphi}(p))$ is the (ordinary) Fourier transform of $(A^*\psi, \varphi(x)) = (\psi, A\varphi(x))$, so by the Plancherel theorem

$$\int |(\psi, A\hat{\varphi}(p))|^2 \, dp = \int |(\psi, A\varphi(x))|^2 \, dx$$

(32) follows by summing over ψ in an orthonormal basis. Next let A be self-adjoint and let $\{E_\Omega\}$ be its family of spectral projections. Then $AE_{(-a,a)}$ is bounded so

$$\int \|AE_{(-a,a)}\hat{\varphi}(p)\|^2 \, dp = \int \|AE_{(-a,a)}\varphi(x)\|^2 \, dx$$

Suppose that one of the integrals in (32) is finite—without loss suppose the right-hand side is finite. Then $\varphi(x) \in D(A)$ a.e. in x, so $\|AE_{(-a,a)}\varphi(x)\|^2$ converges monotonically to $\|A\varphi(x)\|^2$ as $a \to \infty$. Thus,

$$\int \lim_{a\to\infty} \|AE_{(-a,a)}\hat{\varphi}(p)\|^2 \, dp = \int \|A\varphi(x)\|^2 \, dx < \infty$$

In particular, $\lim_{a\to\infty} \|AE_{(-a,a)}\hat{\varphi}(p)\|^2 < \infty$ a.e. in p. It follows that $\hat{\varphi}(p) \in D(A)$ a.e. and (32) holds. Finally, let A be an arbitrary closed operator. By Theorem VIII.32, there is a self-adjoint operator $|A|$ with $D(|A|) = D(A)$ and $\||A|\psi\| = \|A\psi\|$. Thus (32) follows from the case where A is self-adjoint. ∎

Example 1 Let $H = -i\, d/dx$ on $L^2(\mathbb{R})$ so that $(e^{-iHt}\varphi)(x) = \varphi(x - t)$. Let g be in $L^2(\mathbb{R})$ and let A be multiplication by g. By a change of variables, $\int |g(x)\varphi(x - t)|^2 \, dx \, dt = \|g\|_2^2 \|\varphi\|_2^2$ so, by Fubini's theorem, for any $\varphi \in L^2$, and almost all t, $e^{-iHt}\varphi \in D(A)$ and $\int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt = \|g\|_2^2 \|\varphi\|_2^2$. Fix $\varepsilon > 0$; then

$$\int_0^\infty e^{-\varepsilon t} e^{i\lambda t} e^{-iHt}\varphi \, dt = -iR(\lambda + i\varepsilon)\varphi$$

Thus, by the lemma

$$\int_{-\infty}^{\infty} \|AR(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = 2\pi \int_0^{\infty} e^{-2\varepsilon t} \|Ae^{-itH}\varphi\|^2 \, dt$$

Using a similar computation for $\lambda - i\varepsilon$, we see that

$$\int_{-\infty}^{\infty} (\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2) \, d\lambda = 2\pi \int_{-\infty}^{\infty} e^{-2\varepsilon|t|} \|Ae^{-itH}\varphi\|^2 \, dt \tag{33}$$

(33) and the bound on $\int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt$ imply that g is H-smooth and $\|g\|_H = (2\pi)^{-1/2}\|g\|_2$.

Example 2 Let H be any self-adjoint operator and let $A = I$, the identity operator. Again, we use Lemma 1 to conclude that

$$\int_{-\infty}^{\infty} \|R(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = 2\pi \int_0^{\infty} e^{-2\varepsilon t} \|e^{-itH}\varphi\|^2 \, dt = \pi\varepsilon^{-1}\|\varphi\|^2 \tag{34}$$

so that $\sup_{\varepsilon>0} \int_{-\infty}^{\infty} \|R(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = \infty$ for any $\varphi \neq 0$. Thus I is never an H-smooth operator.

One reformulation of H-smoothness is in terms of the unitary group e^{itH}. As an immediate consequence of (33) we have:

Lemma 2 A is H-smooth if and only if for all $\varphi \in \mathscr{H}$, $e^{itH}\varphi \in D(A)$ for almost every $t \in \mathbb{R}$ and for some constant C,

$$\int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt \leq C\|\varphi\|^2$$

C can be chosen equal to $(2\pi)\|A\|_H^2$ and no smaller.

This lemma has several important consequences:

Theorem XIII.22 If A is H-smooth, then A is H-bounded with relative bound zero.

Proof Let $\psi \in D(A^*)$. By the resolvent formula

$$-i(A^*\psi, R(\lambda + i\varepsilon)\varphi) = \int_0^{\infty} (A^*\psi, e^{-iHt}\varphi)e^{i\lambda t}e^{-\varepsilon t} \, dt$$

Thus, by the Schwarz inequality

$$|(A^*\psi, R(\lambda + i\varepsilon)\varphi)|^2 \leq \frac{1}{2\varepsilon}\int_0^\infty |(A^*\psi, e^{-iHt}\varphi)|^2\, dt$$

$$\leq \frac{1}{2\varepsilon}\|\psi\|^2 \int_0^\infty \|Ae^{-iHt}\varphi\|^2\, dt$$

$$\leq \frac{\pi}{\varepsilon}\|A\|_H^2\|\psi\|^2\|\varphi\|^2$$

by Lemma 2. Thus, $R(\lambda + i\varepsilon)\varphi \in D(A^{**}) = D(A)$ and $\|AR(\lambda + i\varepsilon)\|^2 \leq (\pi/\varepsilon)\|A\|_H^2$. We conclude that $D(H) \subset D(A)$ and for $\psi \in D(H)$

$$\|A\psi\| \leq \pi^{1/2}\|A\|_H(\varepsilon^{-1/2}\|H\psi\| + \varepsilon^{1/2}\|\psi\|)$$

Since ε is arbitrary, the theorem is proven. ∎

For a strengthening of Theorem XIII.22, see Problem 49.

Theorem XIII.23 If A is H-smooth, then $\mathrm{Ran}(A^*) \subset \mathscr{H}_{\mathrm{ac}}(H)$.

Proof Since $\mathscr{H}_{\mathrm{ac}}(H)$ is closed, we need only show $\mathrm{Ran}(A^*) \subset \mathscr{H}_{\mathrm{ac}}(H)$. Let $\varphi \in D(A^*)$, $\psi = A^*\varphi$, and let $d\mu_\psi$ be the spectral measure for H associated with ψ. Define

$$F(t) = (2\pi)^{-1/2}\int e^{-itx}\, d\mu_\psi(x) = (2\pi)^{-1/2}(A^*\varphi, e^{-itH}\psi)$$

Then $|F(t)| \leq (2\pi)^{-1/2}\|\varphi\|\,\|Ae^{-itH}\psi\|$, so by Lemma 2, $F \in L^2(\mathbb{R})$. By the Plancherel theorem, $\check{F} \in L^2$ so $d\mu_\psi = \check{F}\, dx$ is absolutely continuous with respect to Lebesgue measure. ∎

It is an instructive exercise to prove Theorem XIII.23 using Theorem XIII.20 and the direct definition of H-smoothness. See also condition (5) of Theorem XIII.25 below. Lemma 2 has important consequences for scattering theory.

Theorem XIII.24 Let H and H_0 be self-adjoint operators. Suppose that $H = H_0 + \sum_{i=1}^n A_i^*B_i$ in the following sense:

(1) $D(H) \subset D(A_i)$; $D(H_0) \subset D(B_i)$; $i = 1, \ldots, n$.
(2) If $\varphi \in D(H)$ and $\psi \in D(H_0)$, then

$$(H\varphi, \psi) = (\varphi, H_0\psi) + \sum_{i=1}^n (A_i\varphi, B_i\psi) \tag{35}$$

If each A_i is H-smooth and each B_i is H_0-smooth, then the wave operators $s\text{-}\lim_{t \to \mp\infty} e^{iHt}e^{-iH_0t}$ exist and are unitary.

Proof Suppose first that $n = 1$. Let $\varphi \in D(H_0)$, $w(t) = e^{iHt}e^{-iH_0t}\varphi$, and $\psi \in D(H)$. Then $(\psi, w(t))$ is differentiable and

$$\frac{d}{dt}(\psi, w(t)) = i(Ae^{-iHt}\psi, Be^{-iH_0t}\varphi)$$

Therefore, if $t > s$,

$$\begin{aligned} |(\psi, w(t) - w(s))| &= \int_s^t |(Ae^{-i\tau H}\psi, Be^{-iH_0\tau}\varphi)| \, d\tau \\ &\leq \left(\int_{-\infty}^{\infty} \|Ae^{-i\tau H}\psi\|^2 \, d\tau\right)^{1/2} \left(\int_s^t \|Be^{-iH_0\tau}\varphi\|^2 \, d\tau\right)^{1/2} \end{aligned}$$

Since ψ is an arbitrary element of $D(H)$,

$$\|w(t) - w(s)\| \leq \sqrt{2\pi}\, \|A\|_H \left(\int_s^t \|Be^{-iH_0\tau}\varphi\|^2 \, d\tau\right)^{1/2}$$

Since the integrand on the right-hand side of the last equation is in $L^1(\mathbb{R})$, this last estimate shows that $w(s)$ is Cauchy as $s \to +\infty$ or as $s \to -\infty$. As a result, the limits exist on a dense set and so on all of $\mathscr{H}$. Since we also have $H_0 = H - B^*A$ by symmetry, the s-lim $e^{iH_0t}e^{-iHt}$ exist and so are unitary. The proof is similar for $n > 1$. ∎

Notice that the limit in Theorem XIII.24 does *not* involve $P_{ac}(H_0)$ (see Section XI.3 for comparison). Thus, if $H_0\psi = E\psi$, then $H\psi = E\psi$. This follows directly from the hypothesis, for $\text{Ran}(B^*) \subset \mathscr{H}_{ac}(H_0)$ implies that $\mathscr{H}_{pp}(H_0) \subset \text{Ker}(B)$, which implies that $H\psi = H_0\psi$.

As a final result in the general theory, we prove that a variety of forms of smoothness are equivaent.

Theorem XIII.25 Let A be a closed operator and let H be a self-adjoint operator. Then the following are equivalent:

(0) A is H-smooth.
(1) For all $\varphi \in \mathscr{H}$, $e^{-itH}\varphi \in D(A)$ for almost all t and

$$c_1 = \sup_{\|\varphi\|=1} \frac{1}{2\pi} \int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt < \infty$$

(2) $D(H) \subset D(A)$ and

$$c_2 = \sup_{\substack{\|\varphi\| = 1 \\ -\infty < a < b < \infty}} \frac{\|AE_{(a,\,b]}\varphi\|^2}{|b-a|} < \infty$$

where E_Ω is the spectral family for H.

(3) $$c_3 = \sup_{\substack{\|\varphi\| = 1;\ \varphi \in D(A^*) \\ -\infty < a < b < \infty}} \frac{\|E_{(a,\,b]}A^*\varphi\|^2}{|b-a|} < \infty$$

(4) $$c_4 = \frac{1}{2\pi} \sup_{\substack{\mu \notin \mathbb{R};\ \varphi \in D(A^*) \\ \|\varphi\| = 1}} |(A^*\varphi, [R(\mu) - R(\bar{\mu})]A^*\varphi)| < \infty$$

(5) $$c_5 = \frac{1}{\pi} \sup_{\substack{\mu \notin \mathbb{R};\ \varphi \in D(A^*) \\ \|\varphi\| = 1}} \|R(\mu)A^*\varphi\|^2 |\operatorname{Im} \mu| < \infty$$

(6) $D(H) \subset D(A)$ and

$$c_6 = \frac{1}{\pi} \sup_{\mu \notin \mathbb{R},\ \|\varphi\| = 1} \|AR(\mu)\varphi\|^2 |\operatorname{Im} \mu| < \infty$$

(7) $D(H) \subset D(A)$ and

$$c_7 = \frac{1}{\pi} \sup_{\mu \notin \mathbb{R},\ \|\varphi\| = 1} (\|AR(\mu)\varphi\|^2 + \|AR(\bar{\mu})\varphi\|^2) |\operatorname{Im} \mu| < \infty$$

Moreover, if any (and thus all) of $c_1 - c_7$ are finite, then all c_i equal $\|A\|_H^2$.

Before proving the theorem, we note that in conditions (5) and (6) one may replace the sup over $\mathbb{C}\backslash\mathbb{R}$ by a sup over $0 < \operatorname{Im} \mu < \alpha$ for any $\alpha > 0$. In the original definition one may replace $\varepsilon > 0$ by $0 < \varepsilon < \alpha$. This follows from the details of the proof if one notes (by (33)) that the expression in (31) is monotone increasing as ε decreases.

The following condition, which is stronger than smoothness, comes from condition (4).

Corollary If $AR(\mu)A^*$ is bounded for each $\mu \notin \mathbb{R}$ in the sense that

$$\sup_{\substack{\psi,\,\varphi \in D(A^*) \\ \|\psi\| = \|\varphi\| = 1}} |(A^*\varphi,\, R(\mu)A^*\psi)| < \infty \qquad \text{and} \qquad \Gamma \equiv \sup_{\mu \notin \mathbb{R}} \|AR(\mu)A^*\| < \infty$$

then A is H-smooth and $\|A\|_H \leq \Gamma/\pi$.

Proof of Theorem XIII.25 We first note that for every closed operator A, every bounded operator B, every $\varphi \in D(A)$, and $\psi \in \mathscr{H}$, we have

$$(\psi, BA\varphi) = (B^*\psi, A\varphi)$$

It follows that $\|BA\varphi\| \leq c\|\varphi\|$ for all $\varphi \in D(A)$ if and only if Ran $B^* \subset D(A^*)$ and $\|A^*B^*\| \leq c$. As a consequence $c_2 = c_3$ and $c_5 = c_6$. Moreover, since $(A^*\varphi,\ [R(\mu) - R(\bar{\mu})]A^*\varphi) = 2 \operatorname{Im} \mu \|R(\mu)A^*\varphi\|^2$, $c_5 = c_4$. Further, $c_0 = c_1$ by Lemma 2. Thus we need only prove that $c_0 = c_3 = c_4 = c_7$ where $c_0 \equiv \|A\|_H^2$. We shall show that

$$c_0 \leq c_4 \leq c_3 \leq c_0 \qquad \text{and} \qquad c_3 \leq c_7 \leq c_1 .$$

$c_0 \leq c_4$: $(2\pi i)^{-1}[R(\mu) - R(\bar{\mu})] = \pi^{-1}(\operatorname{Im} \mu)R(\bar{\mu})R(\mu) \geq 0$ if $\operatorname{Im} \mu > 0$. Let $K(\mu)$ be its positive square root. By the definition of c_4, $\|K(\mu)A^*\varphi\|^2 \leq c_4\|\varphi\|^2$ if $\varphi \in D(A^*)$. Thus, if $c_4 < \infty$, the remark above implies that Ran $K(\mu) \subset D(A)$ and $\|AK(\mu)\|^2 \leq c_4$. Therefore

$$\int_{-\infty}^{\infty} \|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi\|^2 \, d\lambda$$

$$= 4\pi^2 \int_{-\infty}^{\infty} \|AK(\lambda + i\varepsilon)K(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda$$

$$\leq 4\pi^2 c_4 \int_{-\infty}^{\infty} \|K(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda$$

$$= 4\pi^2 c_4 \frac{1}{2\pi i} \int_{-\infty}^{\infty} (\varphi, [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi) \, d\lambda$$

$$= 4\pi^2 c_4 \|\varphi\|^2$$

since in terms of the spectral measure $d\mu_\varphi$ for H,

$$(2\pi i)^{-1} \int_{-\infty}^{\infty} (\varphi, [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi) \, d\lambda$$

$$= \frac{\varepsilon}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{(x - \lambda)^2 + \varepsilon^2} \, d\mu_\varphi(x) \, d\lambda$$

$$= \int_{-\infty}^{\infty} d\mu_\varphi(x) = \|\varphi\|^2$$

Further,

$$[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi = i \int_{-\infty}^{\infty} e^{-\varepsilon|t|} e^{i\lambda t} e^{-iHt} \varphi \, dt$$

so Lemma 1 implies that

$$\int_{-\infty}^{\infty} \|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi\|^2 \, d\lambda = 2\pi \int_{-\infty}^{\infty} e^{-2\varepsilon|t|} \|Ae^{-iHt}\varphi\|^2 \, dt \quad (36)$$

so $c_0 = c_1 \leq c_4$.

$c_4 \leq c_3$: Let $\varphi \in D(A^*)$ and let $d\mu_{A^*\varphi}$ be the spectral measure for H with respect to $A^*\varphi$. Then, by (3)

$$d\mu_{A^*\varphi}(a, b] \leq c_3 |b - a| \, \|\varphi\|^2$$

If I is an arbitrary Borel set, let $|I|$ be its Lebesgue measure. It follows that $d\mu_{A^*\varphi}(I) \leq c_3 |I| \, \|\varphi\|^2$ for arbitrary I, for it is true for open sets and thus by outer regularity for arbitrary sets. Therefore $d\mu_{A^*\varphi}$ is absolutely continuous w.r.t. dx and the Radon–Nikodym derivative $g(x)$ obeys $\|g\|_\infty \leq c_3 \|\varphi\|^2$. Thus if $\mu = \lambda + i\varepsilon$, then

$$|(A^*\varphi, [R(\mu) - R(\bar{\mu})]A^*\varphi)| = \int_{-\infty}^{\infty} \frac{2|\varepsilon|}{(x - \lambda)^2 + \varepsilon^2} g(x) \, dx$$

$$\leq \|g\|_\infty \int_{-\infty}^{\infty} \frac{2|\varepsilon|}{(x - \lambda)^2 + \varepsilon^2} \, dx \leq c_3(2\pi)\|\varphi\|^2$$

We conclude that $c_4 \leq c_3$.

$c_3 \leq c_0$: Let $\varphi \in D(A^*)$. Suppose that a and b are not eigenvalues of H. By Stone's formula,

$$|(A^*\varphi, E_{(a,b]}\psi)|^2$$

$$= \frac{1}{4\pi^2} \lim_{\varepsilon \downarrow 0} \left| \int_a^b (A^*\varphi, [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\psi) \, d\lambda \right|^2$$

$$\leq \frac{1}{4\pi^2} \|\varphi\|^2 \, |b - a| \lim_{\varepsilon \downarrow 0} \int_{-\infty}^{\infty} \|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\psi\|^2 \, d\lambda$$

$$\leq |b - a| \, \|A\|_H^2 \, \|\varphi\|^2 \, \|\psi\|^2$$

In the last step we have used (36). If a and/or b are eigenvalues, $a + \delta$ and $b + \delta$ are not eigenvalues for almost all small δ and $E_{(a,b]} = s\text{-}\lim_{\delta \to 0} E_{(a+\delta, b+\delta]}$ so we see that $c_3 \leq c_0$.

$c_3 \leq c_7$: We already know that $c_3 = c_6$, and $c_6 \leq c_7$ is obvious.

$c_7 \leq c_1$: This is essentially the argument used in the proof of Theorem XIII.22. For by that argument,

$$|(A^*\psi, R(\lambda + i\varepsilon)\varphi)|^2 \leq \frac{1}{2\varepsilon} \|\psi\|^2 \int_0^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt$$

so

$$\|AR(\lambda + i\varepsilon)\varphi\|^2 \leq \frac{1}{2\varepsilon}\int_0^\infty \|Ae^{-iHt}\varphi\|^2\, dt$$

A similar argument for $R(\lambda - i\varepsilon)$ proves that

$$\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2 \leq \frac{1}{2\varepsilon}\int_{-\infty}^\infty \|Ae^{-iHt}\varphi\|^2\, dt$$

Thus $c_7 \leq c_1$. ∎

Notice that criterion (3) provides another proof that $\mathrm{Ran}(A^*) \subset \mathscr{H}_{\mathrm{ac}}(H)$ if A is H-smooth, and that criterion (6) implies Theorem XIII.22. The equality of c_6 and c_7 at first sight seems very mysterious. Some of this mystery can be removed by looking at the proof of a closely related equality:

$$\sup_{\substack{\varepsilon>0\\ \|\varphi\|=1}} \int_{-\infty}^\infty \|AR(\lambda + i\varepsilon)\varphi\|^2\, d\lambda = \sup_{\substack{\varepsilon>0\\ \|\varphi\|=1}} \left\{\int_{-\infty}^\infty (\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2)\, d\lambda\right\}$$

By (33), this equality is equivalent to

$$\sup_{\|\varphi\|=1} \int_0^\infty \|Ae^{-itH}\varphi\|^2\, dt = \sup_{\|\varphi\|=1} \int_{-\infty}^\infty \|Ae^{-itH}\varphi\|^2\, dt$$

which follows by noting that if $\varphi_s = e^{-isH}\varphi$, then

$$\int_0^\infty \|Ae^{-itH}\varphi_s\|^2\, dt = \int_s^\infty \|Ae^{-itH}\varphi\|^2\, dt$$

converges to $\int_{-\infty}^\infty \|Ae^{-itH}\varphi\|^2\, dt$ as $s \to -\infty$.

Before turning to applications, we give two more examples of smooth operators:

Example 3 Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and let A be multiplication by $V \in R$, the Rollnik class. By the estimate,

$$\begin{aligned}\||V|^{1/2}(H_0 - \lambda)^{-1}|V|^{1/2}\|_{\mathrm{oper}} &\leq \||V|^{1/2}(H_0 - \lambda)^{-1}|V|^{1/2}\|_2 \\ &\leq (4\pi)^{-1}\|V\|_R\end{aligned}$$

and the corollary to Theorem XIII.25, $|A|^{1/2}$ is H-smooth.

Example 4 Let H be multiplication by x on $L^2([\alpha, \beta], dx)$ with $\alpha, \beta \in \mathbb{R}$. Let A be a bounded operator on $\mathscr{H}$ so that A^*A is an integral operator of the form

$$(A^*A\psi)(x) = \int_\alpha^\beta K(x, y)\psi(y)\, dy \tag{37}$$

with $\|K\|_\infty \equiv \operatorname{ess\,sup}_{[\alpha, \beta]\times[\alpha, \beta]} |K(x, y)| < \infty$. Then A is H-smooth with $\|A\|_H \leq \|K\|_\infty^{1/2}$. For, let $(a, b]$ be an interval and $\|\varphi\| = 1$. Then

$$\begin{aligned}
\|AE(a, b]\varphi\|^2 &= (\varphi, E(a, b]A^*AE(a, b]\varphi) \\
&= \int_a^b \int_a^b K(x, y)\overline{\varphi(x)}\varphi(y)\, dx\, dy \\
&\leq \left(\int_a^b \int_a^b |K(x, y)|^2\, dx\, dy\right)^{1/2} \left(\int_a^b \int_a^b |\bar{\varphi}(x)\varphi(y)|^2\, dx\, dy\right)^{1/2} \\
&\leq |b - a|\, \|K\|_\infty \|\varphi\|^2
\end{aligned}$$

By criterion (2), $\|A\|_H \leq \|K\|_\infty^{1/2}$. By further analysis (Problems 50, 51) one can show that for every H-smooth operator A, A^*A is of the form (37) and that $\|A\|_H = \|K\|_\infty^{1/2}$. In particular, we note that the analysis above shows that any integral operator

$$(A\psi)(x) = \int_\alpha^\beta A(x, y)\psi(y)\, dy$$

with $\|A\|_\infty < \infty$ is H-smooth. We have thus found many H-smooth operators and, in particular, H-smooth operators A with $\operatorname{Ker}(A) = \{0\}$. Example 1 is related to this example although the operator H in Example 1 is not bounded. For if $f \in L^2$, then $A =$ multiplication by f has $A^*A =$ multiplication by $g \equiv |f|^2 \in L^1$. Passing to the representation in which $-i\, d/dx$ is diagonal (by using Fourier transform), A^*A is an integral operator with kernel equal to $(2\pi)^{-1/2}\hat{g}(x - y) \in L^\infty$.

We turn now to various applications:

A. Weakly coupled quantum systems

Suppose that H_0 is a positive self-adjoint operator and that C is self-adjoint. If $|C|^{1/2}(H_0 + I)^{-1}|C|^{1/2}$ is a bounded operator with bound a, then for any $\varphi \in D(|C|^{1/2})$, $\|(H_0 + I)^{-1/2}|C|^{1/2}\varphi\|^2 \leq a\|\varphi\|^2$ so

$(H_0 + I)^{-1/2}|C|^{1/2}$ is bounded. Taking adjoints, $Q(H_0) \subset Q(C)$ and $\| |C|^{1/2}(H_0 + I)^{-1/2}\|^2 \leq a$. It follows that $(\varphi, |C|\varphi) \leq a(\varphi, (H_0 + I)\varphi)$ for all $\varphi \in Q(H_0)$. Thus C is H_0-form bounded and if $a < 1$, the form sum $H = H_0 + C$ is self-adjoint. Such form sums are the subject of the following theorem.

Theorem XIII.26 (Kato's smoothness theorem) Let H_0 be a positive self-adjoint operator on a Hilbert space $\mathscr{H}$ and let $C_1, \ldots, C_n$ be self-adjoint operators with

$$\alpha_{ij} \equiv \sup_{\mu \notin \mathbb{R}} \| |C_i|^{1/2}(H_0 - \mu)^{-1}|C_j|^{1/2}\| < \infty$$

Suppose that $\{\alpha_{ij}\}_{1 \leq i, j \leq n}$ is the matrix of an operator of norm less than 1 on $\mathbb{C}^n$ (with the natural Hilbert space norm). Then:

(a) The form sum $H = H_0 + \sum_{i=1}^n C_i$ is a closed form on $Q(H_0)$.
(b) The wave operators s-$\lim_{t \to \mp\infty} e^{iHt}e^{-iH_0t}$ exist and are unitary.

In particular, H and H_0 are unitarily equivalent operators.

Proof Introduce the Hilbert space $\mathscr{H}' = \oplus_{i=1}^n \mathscr{H}_i$ where each $\mathscr{H}_i$ is a copy of $\mathscr{H}$. By the discussion preceding the theorem and the hypothesis $\alpha_{ii} < \infty$, we have that each $|C_i|$ is H_0-form bounded, so that $|C_i|^{1/2}$ is defined from $Q(H_0)$ to $\mathscr{H}$. As a result, we can define B: $Q(H_0) \to \mathscr{H}'$ by $(B\psi)_i = |C_i|^{1/2}\psi$. The hypothesis of the theorem implies that

$$\alpha \equiv \sup_{\mu \notin \mathbb{R}} \| B(H_0 - \mu)^{-1}B^* \| < 1 \tag{38}$$

Let $B = U|B|$ be the polar decomposition of B. Then, since $|B| = U^*B$ and U is a partial isometry, (38) implies that $|B|(H_0 + I)^{-1}|B|$ is a bounded operator of norm smaller than α. Again, it follows from the argument preceding the theorem that

$$(\varphi, |B|^2\varphi) \leq \alpha(\varphi, (H_0 + I)\varphi)$$

or that

$$\left(\varphi, \sum_{i=1}^n |C_i|\varphi\right) \leq \alpha(\varphi, (H_0 + I)\varphi) \tag{39}$$

From (39), we conclude that $\sum_{i=1}^n C_i$ is H_0-form bounded with relative bound $\alpha < 1$ proving (a).

Next, we note that for $\mu \notin [0, \infty)$,

$$(H-\mu)^{-1} = (H_0-\mu)^{-1} - \sum_{n=0}^{\infty}(-1)^n(H_0-\mu)^{-1}B^*W(B(H_0-\mu)^{-1}B^*W)^nB(H_0-\mu)^{-1} \tag{40}$$

where W: $\mathscr{H}' \to \mathscr{H}'$ by $(W\varphi)_i = (\operatorname{sgn} C_i)\varphi_i$. (40) holds since the sum is convergent by (38) and one checks that, in the language of quadratic forms (Section VIII.6), the right-hand side maps $\mathscr{H}_{-1}$ to $\mathscr{H}_{+1}$ and is an inverse for $(H-\mu)$: $\mathscr{H}_{+1} \to \mathscr{H}_{-1}$. From (40) one easily sees that

$$\sup_{\mu \notin \mathbb{R}} \|B(H-\mu)^{-1}B^*\| \leq \alpha(1-\alpha)^{-1} \tag{41}$$

so each $|C_i|^{1/2}$ and $C_i^{1/2} \equiv |C_i|^{1/2} \operatorname{sgn} C_i$ is H-smooth by the corollary to Theorem XIII.25. Similarly, by the basic hypotheses and that corollary, each $|C_i|^{1/2}$ is H_0-smooth. Thus, by Theorem XIII.24, both s-$\lim_{t \to \mp\infty} e^{iHt}e^{-iH_0t}$ and s-$\lim_{t \to \mp\infty} e^{iH_0t}e^{-iHt}$ exist. These maps are all isometries and inverses of one another. This proves (b). ∎

As an application of this theorem, the reader should prove the strong version of Theorem XIII.21 found in Problem 56. If one does not want to worry about detailed estimates, it is often useful to state Kato's smoothness theorem in the form:

Corollary Let H_0 be self-adjoint and positive. Let $C_1, \ldots, C_n$ be self-adjoint and let $C = \sum_{i=1}^n C_i$. Suppose that for each i and j

$$\sup_{\mu \notin \mathbb{R}} \| |C_i|^{1/2}(H_0-\mu)^{-1}|C_j|^{1/2}\| < \infty$$

Then there exists $\Lambda > 0$ so that for all $\lambda \in (-\Lambda, \Lambda)$:

(a) $H(\lambda) = H_0 + \lambda C$ is a closed form on $Q(H_0)$.
(b) The wave operators $\Omega_\lambda^\pm = \text{s-}\lim_{t \to \mp\infty} e^{itH(\lambda)}e^{-itH_0}$ exist and are unitary.

It is actually possible to prove that $\Omega_\lambda^\pm$ are analytic in λ (see the Notes and Problems 53, 54). Now we can easily handle "weakly coupled" N-body Schrödinger operators.

Theorem XIII.27 (the Iorio–O'Carroll theorem) Let $m \geq 3$, $N \geq 2$. Let $\tilde{H}_0$ be the operator

$$\tilde{H}_0 = \sum_{i=1}^{N} (-2\mu_i)^{-1} \Delta_i$$

on $L^2(\mathbb{R}^{Nm})$ where each $\mu_i > 0$ and $r \in \mathbb{R}^{Nm}$ is written $r = \langle r_1, \ldots, r_N \rangle$ with $r_i \in \mathbb{R}^m$. Let H_0 be $\tilde{H}_0$ with the center of mass motion removed (see Section XI.5). Let $V = \sum_{i<j} V_{ij}(r_i - r_j)$ where each $V_{ij} \in L^{m/2+\varepsilon}(\mathbb{R}^m) \cap L^{m/2-\varepsilon}(\mathbb{R}^m)$ for some fixed $\varepsilon > 0$. Then for all $\lambda \in \mathbb{R}$ with $|\lambda|$ sufficiently small, $H_0 + \lambda V$ (defined as a form sum) is unitarily equivalent to H_0. The wave operators provide unitary equivalence. In particular, $H_0 + \lambda V$ has no bound states, no singular spectrum and has complete scattering.

Before proving the Iorio–O'Carroll theorem, we make several remarks. First, it is merely for contact with the notions of N-body quantum theory that we remove the center of mass motion. Secondly, we note that only when $m = 3$ is the form sum necessary. If $m \geq 4$, Theorem X.20 tells us that the operator sum $H_0 + \lambda V$ is self-adjoint on $C_0^\infty(\mathbb{R}m(N-1)$ if λ is real. Thirdly, we note that, by Theorem XIII.11, there can be no weak coupling theorem when $m = 1$ or 2, but there is a result on $L^2([0, \infty))$ (Problem 58). Finally, the conditions on V_{ij} cannot be weakened much; for if V_{ij} has non-$L^{m/2}$ local singularities at finite points (e.g., $r^{-2-\varepsilon}$ behavior at $r = 0$), then self-adjointness is lost and if V_{ij} has non-$L^{m/2}$ behavior at infinity (e.g., only $r^{-2+\varepsilon}$ falloff at ∞), then it can happen that $H_0 + \lambda V$ has bound states no matter how small λ is (see Theorem XIII.6).

Proof of Theorem XIII.27 Consider first the case $N = 2$. Then $H_0 = (-2\nu)^{-1} \Delta$ on $L^2(\mathbb{R}^m)$, so by Theorem IX.30,

$$\|e^{-iH_0 t}\varphi\|_r \leq (ct)^{-m[\frac{1}{2}-r^{-1}]} \|\varphi\|_{r'} \tag{42}$$

where $2 \leq r \leq \infty$, $r^{-1} + r'^{-1} = 1$ and c is chosen suitably. Thus, if $f \in L^p$ and $p > 2$, then by Hölder's inequality and (42)

$$\|fe^{-iH_0 t} f\varphi\|_2 \leq (ct)^{-mp^{-1}} \|f\|_p^2 \|\varphi\|_2 \tag{43}$$

Thus, if $f \in L^{m-\varepsilon} \cap L^{m+\varepsilon}$ (and $m > 2 + \varepsilon$),

$$\int_{-\infty}^{\infty} \|fe^{-iH_0 t} f\varphi\|_2 \, dt \leq d(\|f\|_{m+\varepsilon} + \|f\|_{m-\varepsilon})^2 \|\varphi\|_2$$

for a suitable constant d. Since

$$f(H_0 - z)^{-1} f\varphi = i \int_0^\infty e^{izt}(fe^{-iH_0 t} f)\varphi \, dt$$

if Im $z > 0$, we conclude that

$$\|f(H_0 - z)^{-1} f\varphi\|_2 \leq d(\|f\|_{m+\varepsilon} + \|f\|_{m-\varepsilon})^2 \|\varphi\|_2$$

if Im $z > 0$. A similar argument holds if Im $z < 0$. Letting $f = |V|^{1/2}$, we conclude that

$$\sup_{z \notin \mathbb{R}} \| |V|^{1/2} (H_0 - z)^{-1} |V|^{1/2} \| < \infty$$

The theorem (in case $N = 2$) then follows from the corollary to Theorem XIII.26.

To prove the theorem in the general case, we need only prove that

$$\sup_{z \notin \mathbb{R}} \| |V_{ij}|^{1/2} (H_0 - z)^{-1} |V_{k\ell}|^{1/2} \| < \infty$$

for all i, j, k, ℓ and apply the corollary to Theorem XIII.26. It is necessary to consider three distinct cases:

Case 1 $(ij) = (k\ell)$ Without loss of generality suppose that $i = k = 1$ and $j = \ell = 2$. Let $H_0^{(12)} = (-2\mu_{12})^{-1} \Delta_{12}$ where $\mu_{12}^{-1} = \mu_1^{-1} + \mu_2^{-1}$ and Δ_{12} is the Laplacian with respect to r_{12} in a Jacobi coordinate system (see Section XI.5). Thus, $H_0 - H_0^{(12)}$ depends only on the remaining Jacobi coordinates $\zeta_2, \ldots, \zeta_{N-1}$ and so commutes with any function of $\zeta_1 = r_2 - r_1$. If $f \in L^p(\mathbb{R}^m)$ and f_1 is multiplication by $f(\zeta_1)$, then

$$\|f_1 e^{-itH_0} f_1 \varphi\|_2 = \|f_1 e^{-itH_0^{(12)}} f_1 \varphi\|_2 \tag{44}$$

Let $\varphi \in \mathscr{S}(\mathbb{R}^{m(N-1)})$. By the basic two-body estimate (43),

$$\int |f_1(e^{-iH_0^{(12)}t} f_1 \varphi(\zeta_1, \zeta_2, \ldots, \zeta_{N-1})|^2 \, d\zeta_1 \leq (ct)^{-2mp^{-1}} \|f\|_p^4 \int |\varphi(\zeta)|^2 \, d\zeta_1$$

Integrating over $\zeta_2, \ldots, \zeta_{N-1}$ and using (44) we see that (43) still holds. Thus, by mimicking the two-body proof,

$$\sup_{z \notin \mathbb{R}} \| |V_{12}|^{1/2} (H_0 - z)^{-1} |V_{12}|^{1/2} \| < \infty$$

Case 2 $j = k$; i, j, ℓ distinct Without loss of generality, suppose that $i = 1; j = k = 2; \ell = 3$. Again use Jacobi coordinates with $\zeta_1 = r_2 - r_1$ and with $r_{23} = \alpha\zeta_1 + \beta\zeta_2$ (with $\alpha, \beta \neq 0$). Since $H_0 - H_0^{(12)}$ commutes with functions of ζ_1:

$$\| |V_{12}|^{1/2} e^{-itH_0} |V_{23}|^{1/2} \varphi \| = \| |V_{12}|^{1/2} e^{-itH_0^{(12)}} |V_{23}|^{1/2} \varphi \|$$

Fix $\zeta' \equiv \langle \zeta_2, \ldots, \zeta_{N-1} \rangle$ and let $\varphi \in \mathscr{S}(\mathbb{R}^{m(N-1)})$. Then by the basic two-body estimate (43),

$$\int |V_{12}(\zeta_1)|\,|e^{-itH_0^{(12)}} V_{23}^{1/2}(\alpha\zeta_1 - \beta\zeta_2)\varphi(\zeta_1, \zeta')|^2\, d\zeta_1$$

$$\leq (ct)^{-2mp^{-1}} \|V_{12}\|_{p/2} \|V_{23}\|_{p/2} \alpha^{-2m/p} \int |\varphi(\zeta)|^2\, d\zeta_1$$

where we have used the fact that

$$\int |V_{23}(\alpha\zeta_1 - \beta\zeta_2)|^{p/2}\, d\zeta_1 = \alpha^{-1} \int |V_{23}(x)|^{p/2}\, dx$$

independently of ζ_2. Integrating over ζ', we find that

$$\| |V_{12}|^{1/2} e^{-itH_0^{(12)}} |V_{23}|^{1/2} \varphi\|_2^2 \leq \alpha^{-2/p}(ct)^{-2mp^{-1}} \|V_{12}\|_{p/2} \|V_{23}\|_{p/2} \|\varphi\|_2^2$$

From this estimate, it follows that

$$\sup_{z \notin \mathbb{R}} \| |V_{12}|^{1/2} (H_0 - z)^{-1} |V_{23}|^{1/2} \| < \infty$$

as in the two-body case.

Case 3 i, j, k, ℓ *all distinct* Without loss of generality suppose that $i = 1, j = 2, k = 3, \ell = 4$. Then,

$$\begin{aligned} &|(\varphi, |V_{12}|^{1/2} e^{-itH_0} |V_{34}|^{1/2} \psi)| \\ &\quad = |(e^{+itH_0^{(34)}} \varphi, |V_{12}|^{1/2} e^{-it(H_0 - H_0^{(34)})} |V_{34}|^{1/2} \psi)| \\ &\quad = |(|V_{34}|^{1/2} e^{itH_0^{(34)}} \varphi, |V_{12}|^{1/2} e^{-it(H_0 - H_0^{(34)})} \psi)| \\ &\quad \leq \| |V_{34}|^{1/2} e^{itH_0^{(34)}} \varphi\| \, \| |V_{12}|^{1/2} e^{-itH_0^{(12)}} \psi\| \end{aligned}$$

In the first step, we have used the fact that $|V_{12}|^{1/2}$ and $H_0^{(34)}$ commute; in the second step that $|V_{34}|^{1/2}$ commutes with $H_0 - H_0^{(34)}$ and $|V_{12}|^{1/2}$; and in the final step that $|V_{12}|^{1/2}$ and $H_0 - H_0^{(34)} - H_0^{(12)}$ commute. By step (1) and the corollary to Theorem XIII.25, $|V_{ij}|^{1/2}$ is $H_0^{(ij)}$-smooth. Thus,

$$\begin{aligned} &\int_{-\infty}^{\infty} \| |V_{34}|^{1/2} e^{+itH_0^{(34)}} \varphi\| \, \| |V_{12}|^{1/2} e^{-itH_0^{(12)}} \psi\| \, dt \\ &\quad \leq \left(\int_{-\infty}^{\infty} \| |V_{34}|^{1/2} e^{itH_0^{(34)}} \varphi\|^2 \, dt \right)^{1/2} \\ &\quad \times \left(\int_{-\infty}^{\infty} \| |V_{12}|^{1/2} e^{-itH_0^{(12)}} \psi\|^2 \, dt \right)^{1/2} \\ &\quad \leq \| |V_{34}|^{1/2} \|_{H_0^{(34)}} \, \| |V_{12}|^{1/2} \|_{H_0^{(12)}} \, \|\varphi\| \, \|\psi\| \end{aligned}$$

so that

$$\int_{-\infty}^{\infty} |(\varphi, |V_{12}|^{1/2} e^{-itH_0} |V_{34}|^{1/2}\psi)| \, dt \leq c\|\varphi\| \, \|\psi\|$$

Since

$$(\varphi, |V_{12}|^{1/2}(H_0 - z)^{-1} |V_{34}|^{1/2}\psi)$$
$$= -i \int_0^{\infty} e^{izt}(\varphi, |V_{12}|^{1/2} e^{-iH_0 t} |V_{23}|^{1/2}\psi) \, dt$$

if Im $z > 0$, we conclude that

$$\sup_{z \notin \mathbb{R}} \| |V_{12}|^{1/2}(H_0 - z)^{-1} |V_{34}|^{1/2}\| < \infty$$

This completes the proof of case 3. ∎

If one of the particles has infinite mass, Case 2 cannot be handled as above since $\alpha = 0$ if $\mu_2 = \infty$. In that event, the method of case 3 will work and the theorem remains true.

B. Positive commutators and repulsive potentials

As a second application of smoothness techniques, we develop a method that will allow us to prove that Hamiltonians with repulsive potentials have purely absolutely continuous spectrum.

Theorem XIII.28 (the Putnam–Kato theorem) Let H and A be bounded self-adjoint operators. Suppose that $C = i[H, A]$ is positive. Then $C^{1/2}$ is H-smooth. In particular, if Ker $C = \{0\}$, then H has purely absolutely continuous spectrum.

Proof The second statement follows from the first by Theorem XIII.23 and the fact that $\text{Ker}(C^{1/2}) = [\text{Ran}(C^{1/2})]^{\perp} = \{0\}$. We compute:

$$\frac{d}{dt} e^{itH} A e^{-itH}\varphi = ie^{itH}[H, A]e^{-itH}\varphi = e^{itH} C e^{-itH}\varphi$$

Thus

$$\int_s^t (\varphi, e^{i\tau H} C e^{-i\tau H}\varphi) \, d\tau = (\varphi, e^{itH} A e^{-itH}\varphi) - (\varphi, e^{isH} A e^{-isH}\varphi)$$

so

$$\int_s^t \|C^{1/2}e^{-i\tau H}\varphi\|^2 \, d\tau \leq 2\|A\| \, \|\varphi\|^2$$

Since t and s are arbitrary, $C^{1/2}$ is H-smooth and

$$\|C^{1/2}\|_H^2 \leq \|A\|/\pi \; \blacksquare$$

For an alternative method of proof, see Problem 59.

Example 5 Since examples of positive commutators are not easy to construct directly, we present examples to show that the hypotheses of Theorem XIII.28 are sometimes obeyed. In fact, there is a sort of converse to the fact that $C^{1/2}$ is H-smooth: If H is bounded and B is any bounded H-smooth operator, there exists a bounded operator A with $i[H, A] = B^*B$. Since there are H-smooth operators with zero kernel when H has purely absolutely continuous spectrum (see Example 4), one can construct many pairs H, A for which the hypotheses of Theorem XIII.28 are obeyed. If B is H-smooth, then by following the argument in Theorem XIII.24, one can show that $\Gamma_H^+(B^*B) \equiv \text{s-lim}_{s\to\infty} \, i \int_0^s e^{itH}B^*Be^{-itH} \, dt$ exists. Now,

$$\begin{aligned}[H, \Gamma_H^+(B^*B)] &= \text{s-lim}_{s\to\infty} \, i \int_0^s e^{itH}[H, B^*B]e^{-itH} \, dt \\ &= \text{s-lim}_{s\to\infty} \, (e^{isH}B^*Be^{-isH} - B^*B) \\ &= -B^*B\end{aligned}$$

where we have used the fact that $e^{itH}B^*Be^{-itH}\varphi \in L^2$ with a uniformly bounded derivative to conclude that $\text{s-lim}_{s\to\infty} \, (e^{isH}B^*Be^{-isH}) = 0$ (Problem 62). Letting $A = i\Gamma_H^+(B^*B)$, we see that $i[H, A] = B^*B$.

We want to apply the idea of positive commutators to prove that N-body Schrödinger operators with repulsive potentials have purely absolutely continuous spectrum. A repulsive potential is a function on $\mathbb{R}^m$ so that $V(r\hat{e}) \leq V(r'\hat{e})$ for each unit vector $\hat{e}$ and all $r > r'$. Thus repulsive potentials tend to push particles apart, so we expect no bound states and thus only absolutely continuous spectra. There is another way of describing the fact that V is repulsive that makes the connection with positive commutators clearer. Let $U(\theta)$ be the family of dilations, $(U(\theta)\psi)(r) = e^{+m\theta/2}\psi(e^\theta r)$. Then $[U(\theta)VU(\theta)^{-1}](r) = V(e^\theta r)$, so repulsive potentials obey the condition

that $V_\theta \equiv U(\theta)VU(\theta)^{-1}$ is monotone decreasing as θ increases. Since $U(\theta)H_0\,U(\theta)^{-1} = e^{-2\theta}H_0$, the kinetic energy also decreases monotonically under dilations. Thus, formally,

$$\frac{d}{d\theta}\,U(\theta)(H_0 + V)U(\theta)^{-1} \leq 0$$

Letting

$$D = \frac{i}{2}\sum_{i=1}^{m}\left(x_i\frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_i}x_i\right)$$

be the generator of $U(\theta)$ (i.e., $U(\theta) = \exp(-i\theta D)$), we see that $i[D, H] \geq 0$ formally.

Physically, there is another way of looking at the fact that $i[D, H] \geq 0$. For $D = -(i/2)[H, x^2]$. Therefore, if one defines the Heisenberg picture moment of inertia

$$I(t) = e^{+iHt}x^2e^{-iHt}$$

then on a formal level $i[D, H] \geq 0$ is equivalent to $\ddot{I}(t) \geq 0$. It is easy to see that classically the repulsive potential obeys this condition and indeed we have used similar ideas in Theorem XI.3.

Theorem XIII.28 is not directly applicable for three reasons: (1) The computations were formal; as usual this requires care with domains and cores, but it turns out that no extra technical assumption is needed. (2) H is not bounded. It turns out that since H is positive, this in itself would not be very serious (see Problem 61). (3) D is not bounded. This is more serious. The d/dx piece of D is not hard to control since it is H-bounded but the factor of x is hard to control directly. In the proof of the theorem below, we will use a cutoff x which will have the effect of making the computations more complicated. Since V being repulsive is related to $dV/dr \leq 0$, it is the derivative in D rather than the x that is important—thus cutting off x will not destroy $i[A, H] \geq 0$.

Theorem XIII.29 (Lavine's theorem) Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^m)$ $(m \geq 3)$. Let V be a function on $\mathbb{R}^m$ so that

(i) Multiplication by V is H_0-bounded with relative bound zero.
(ii) The distributional derivative $\sum_{i=1}^{n} x_i\,\partial V/\partial x_i$ is negative.

Then $H = H_0 + V$ has purely absolutely continuous spectrum.

Proof Choose α obeying $\frac{1}{2} < \alpha < \frac{3}{2}$ and define $g(r) = \int_0^r (1+\rho^2)^{-\alpha}\, d\rho$. Let A be the operator

$$Af = i \sum_{k=1}^{m} \left[x_k \frac{g(r)}{r} \frac{\partial f}{\partial x_k} + \frac{\partial}{\partial x_k}\left(x_k \frac{g(r) f}{r} \right) \right] \tag{45}$$

Since $g(r)r^{-1}$ is C^∞, A maps C_0^∞ into itself. If g were replaced by r in (45), the operator resulting would be the generator of dilations, so (45) is a partially cutoff version of this generator. In fact, A has a direct geometrical interpretation. Let $T_y\colon \mathbb{R}^n \to \mathbb{R}^n$ be defined by the conditions: $T_0(x) = x$, and $y(\gamma) = T_\gamma x$ solves $\dot{y} = |y|^{-1} g(|y|) y$. Then,

$$(e^{-iyA} f)(x) = N_\gamma(x) f(T_\gamma x)$$

where $N_\gamma(x)$ is a normalizing factor (the square root of a Jacobian determinant).

Our first goal is to prove that for some constant $c > 0$,

$$i[A, H] \geq c(1+r^2)^{-\alpha-1}$$

in the sense that for all $\varphi \in C_0^\infty(\mathbb{R}^n)$,

$$i(A\varphi, H\varphi) - i(H\varphi, A\varphi) \geq c(\varphi, (1+r^2)^{-\alpha-1}\varphi) \tag{46}$$

First, we compute

$$\begin{aligned} & i(A\varphi, V\varphi) - i(V\varphi, A\varphi) \\ &= 2 \operatorname{Re} \sum_{i=1}^{m} \int V(x) \left[\overline{\varphi(x)} \left\{ \frac{x_i}{r} g(r) \frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\frac{x_i}{r} g(r) \right) \right\} \varphi(x) \right] dx \\ &= 2 \int V(x) \sum_{i=1}^{m} \frac{\partial}{\partial x_i} x_i \left(\frac{g(r)}{r} |\varphi(x)|^2 \right) dx \geq 0 \end{aligned}$$

by hypothesis (ii). Thus we need only verify (46) when $V = 0$, a tedious but not too difficult task. As a preliminary, we note that for all r,

$$rg'(r) - g(r) \leq 0 \tag{47a}$$

$$g''(r) = -2\alpha r(1+r^2)^{-\alpha-1} \tag{47b}$$

$$g'''(r) + (2\alpha+1)r^{-1}g''(r) \leq 0 \tag{47c}$$

To prove (47a), we remark that $(1+r^2)^{-\alpha}$ is monotone decreasing, so its average value $g(r)r^{-1} = r^{-1}\int_0^r (1+\rho^2)^{-\alpha}\, d\rho$ is also monotone decreasing. Since $rg' - g = r^2(r^{-1}g)'$, (47a) is proven. (47b) and (47c) follow from the explicit calculations:

$$g''(r) = -2\alpha r(1+r^2)^{-\alpha-1}$$

$$g'''(r) + (2\alpha+1)r^{-1}g''(r) = -4\alpha(\alpha+1)(1+r^2)^{-\alpha-2}$$

Next we prove that

$$-\Delta\left(\sum_{j=1}^{m}\frac{\partial g_j}{\partial x_j}\right) \geq c(1+r^2)^{-\alpha-1} \tag{48}$$

where $g_j(x) = x_j r^{-1} g(r)$. For

$$\frac{\partial g_j}{\partial x_k} = r^{-1}g(\delta_{jk} - r^{-2}x_j x_k) + r^{-2}x_j x_k g' \tag{49}$$

Thus

$$\sum_{j=1}^{m}\frac{\partial g_j}{\partial x_j} = (n-1)r^{-1}g + g'$$

Using the fact that for a spherically symmetric function h,

$$\Delta h = r^{-1}(rh)'' + (n-3)r^{-1}h'$$

we find that

$$-\Delta\left(\sum_{j=1}^{n}\frac{\partial g_j}{\partial x_j}\right) = -(g''' + (2\alpha+1)r^{-1}g'') - (2n-2\alpha-3)r^{-1}g''$$
$$-(n-1)(n-3)r^{-3}(rg'-g)$$

Since $n \geq 3$ and $\alpha < \frac{3}{2}$, (48) follows from (47). Finally, we compute on C_0^∞ functions that

$$-\left[g_k\frac{\partial}{\partial x_k}, H_0\right] = \sum_{i=1}^{n}\left[g_k\frac{\partial}{\partial x_k}, \frac{\partial^2}{\partial x_i^2}\right]$$
$$= \sum_{i=1}^{n} 2p_i\frac{\partial g_k}{\partial x_i}p_k + i\frac{\partial^2 g_k}{\partial x_i^2}p_k$$

where $p_k = i^{-1}\,\partial/\partial x_k$. Using

$$-\left[g_k\frac{\partial}{\partial x_k} + \frac{\partial}{\partial x_k}g_k, H_0\right] = -\left[g_k\frac{\partial}{\partial x_k}, H_0\right] - \left[g_k\frac{\partial}{\partial x_k}, H_0\right]^*$$

we see that

$$i[A, H_0] = \sum_{i,k} 2p_k\left(\frac{\partial g_i}{\partial x_k} + \frac{\partial g_k}{\partial x_i}\right)p_i - \Delta\left(\sum_j \frac{\partial g_j}{\partial x_j}\right)$$

Thus by (48) the proof of (46) has been reduced to proving

$$\sum_{i,k} 2p_k\left(\frac{\partial g_i}{\partial x_k} + \frac{\partial g_k}{\partial x_i}\right)p_i \geq 0 \tag{50}$$

By (49) the left-hand side of (50) is

$$4 \sum_{i,k} \{p_k[(r^{-1}g)(\delta_{ik} - r^{-2}x_i x_k)]p_i + p_k(r^{-2}g')x_i x_k p_i\}$$

Fix $x \in \mathbb{R}^n$. Then, by the Schwarz inequality, the matrix $\{\delta_{ik} - r^{-2}x_i x_k\}$ is positive definite. Further, $\{x_i x_k r^{-2}\}$ is clearly positive definite, so (50) holds and this completes the proof of (46).

Next, we need to know that $A << H$, i.e., that A is H-bounded with relative bound zero. Since $V << H_0$ by hypothesis, we need only prove that $A << H_0$. But $\partial/\partial x_i << H_0$, $x_i g r^{-1}$ is bounded, and

$$A = 2i \sum_{i=1}^{n} x_i g r^{-1} \partial/\partial x_i + i(n-1)r^{-1}g + ig'$$

so $A << H_0$ is proven. Since C_0^∞ is a core for H and $A << H$, (46) holds for all $\varphi \in D(H)$.

Now let $\varphi \in D(H)$ and let B be multiplication by $c^{1/2}(1+r^2)^{-(\alpha+1)/2}$. Then we claim that

$$\int_{-\infty}^{\infty} \|Be^{-itH}\varphi\|^2 \, dt \leq d\|(H+I)\varphi\|^2 \tag{51}$$

for a suitable constant d. For, by (46),

$$\begin{aligned}
&\int_{-\infty}^{\infty} \|Be^{-itH}\varphi\|^2 \, dt \\
&\quad = \int_{-\infty}^{\infty} (e^{-itH}\varphi, B^*Be^{-itH}\varphi) \, dt \\
&\quad \leq \int_{-\infty}^{\infty} i\{(Ae^{-itH}\varphi, He^{-itH}\varphi) - (He^{-itH}\varphi, Ae^{-itH}\varphi)\} \, dt \\
&\quad \leq 2 \sup_{-\infty<s<\infty} |(e^{-isH}\varphi, Ae^{-isH}\varphi)| \\
&\quad \leq 2\|\varphi\| \, \|A(H+I)^{-1}\| \, \|(H+I)\varphi\|
\end{aligned}$$

which proves (51).

To conclude the proof we notice that (51) implies that $B(H+I)^{-1}$ is H-smooth. Since $\mathrm{Ran}(B^*)$ and $\mathrm{Ran}(H+I)^{-1}$ are dense, the closure of $\mathrm{Ran}(H+I)^{-1}B^*$ is $\mathscr{H}$. Theorem XIII.23 thus implies that $\mathscr{H} \subset \mathscr{H}_{\mathrm{ac}}$. Therefore H has purely absolutely continuous spectrum. ∎

Corollary Let $m(N-1) \geq 3$. Let $\tilde{H}_0 = \sum_{i=1}^{N} (-2\mu_i)^{-1} \Delta_i$ on $L^2(\mathbb{R}^{Nm})$ and let H_0 be $\tilde{H}_0$ with its center of mass motion removed. For each i, j suppose that V_{ij}: $\mathbb{R}^m \to \mathbb{R}$ and

(i) $V_{ij} \in L^p(\mathbb{R}^m) + L^\infty(\mathbb{R}^m)$ ($p = 2$ if $m \leq 3$, $p > 2$ if $m = 4$; $p = m/2$ if $m \geq 5$).

(ii) $\sum_{k=1}^{m} x_k \, \partial V_{ij}/\partial x_k \leq 0$ in the distributional sense.

Then the operator $H = H_0 + \sum_{i<j} V_{ij}(r_i - r_j)$ on $L^2(\mathbb{R}^{m(N-1)})$ has purely absolutely continuous spectrum.

Proof Let ζ be a Jacobi coordinate system so $H_0 = \sum_{i=1}^{N-1} (-2M_i)^{-1} \Delta_{\zeta_i}$ and let $q_i = (2M_i)^{1/2}\zeta_i$ so $H_0 = -\sum_{i=1}^{N-1} \Delta_{q_i}$. If we can show that $\sum_{i=1}^{N-1} q_i \cdot \nabla_{q_i} V_{jk} \leq 0$ for all j, k, then the result follows from Theorem XIII.29. Suppose first that each V_{jk} is smooth. Then $V_{jk} = V_{jk}(\sum_{i=1}^{N-1} \alpha_i q_i)$ for suitable α_i. So

$$\sum_i q_i \cdot \nabla_{q_i} V_{jk}\left(\sum_\ell \alpha_\ell q_\ell\right) = \left(\sum_i \alpha_i q_i\right) \cdot (\nabla_r V_{jk})(r)\Big|_{r=\sum \alpha_\ell q_\ell} = (r \cdot \nabla_r V_{jk})(r)\Big|_{r=\sum \alpha_\ell q_\ell}$$

This is nonpositive by hypothesis. For arbitrary V_{jk}, we average with test functions and mimic the above argument. ∎

C. Local smoothness and wave operators for repulsive potentials

As a final topic in the theory of smooth operators, we shall discuss an extension of Theorem XIII.24. The "trouble" with that theorem is that its conclusion is too strong—H and H_0 are unitarily equivalent. In particular, the theorem cannot be applied to quantum Hamiltonians that have any pure point spectrum. We thus introduce a weaker notion than smoothness.

Definition Let H be a self-adjoint operator with spectral projections E_Ω. We say that A is **H-smooth on Ω**, a Borel set, if and only if AE_Ω is H-smooth.

Theorem XIII.30 Let H be self-adjoint with resolvent R and spectral projections, $\{E_\Omega\}$. Let $\Omega \subset \mathbb{R}$. Suppose that $D(A) \supset D(H)$ and that *either*

(a) $\sup_{0<|\varepsilon|<1,\, \lambda \in \Omega} |\varepsilon| \, \|AR(\lambda + i\varepsilon)\|^2 < \infty$

or

(b) $\sup_{0<\varepsilon<1,\, \lambda \in \Omega} \|AR(\lambda + i\varepsilon)A^*\| < \infty$

Then A is H-smooth on $\bar{\Omega}$, the closure of Ω.

Proof (a) For each $\varepsilon \neq 0$, $\|AR(\lambda + i\varepsilon)\|$ is continuous in λ, so the bound

$$C = \sup\{|\varepsilon| \|AR(\lambda + i\varepsilon)\|^2 \mid \lambda \in \Omega, 0 < |\varepsilon| < 1\}$$

extends to all $\lambda \in \bar{\Omega}$. Suppose $\lambda \in \mathbb{R}\backslash\bar{\Omega}$. Choose $\lambda_0 \in \bar{\Omega}$ with $|\lambda - \lambda_0| = \text{dist}(\lambda, \bar{\Omega})$. Then

$$\begin{aligned}
&|\varepsilon| \|AR(\lambda + i\varepsilon)E_\Omega \varphi\|^2 \\
&\quad = |\varepsilon| \|AR(\lambda_0 + i\varepsilon)[I - (\lambda_0 - \lambda)R(\lambda + i\varepsilon)]E_{\bar{\Omega}} \varphi\|^2 \\
&\quad \leq |\varepsilon| \|AR(\lambda_0 + i\varepsilon)\|^2 \|(I - (\lambda_0 - \lambda)R(\lambda + i\varepsilon))E_{\bar{\Omega}}\|^2 \|\varphi\|^2 \\
&\quad \leq 4|\varepsilon| \|AR(\lambda_0 + i\varepsilon)\|^2 \|\varphi\|^2
\end{aligned}$$

since $|\lambda_0 - \lambda| \, |x - \lambda + i\varepsilon|^{-1} < 1$ for any $x \in \bar{\Omega}$. Thus

$$\sup_{\substack{\lambda \in \mathbb{R} \\ \varepsilon \neq 0}} |\varepsilon| \|AR(\lambda + i\varepsilon)E_{\bar{\Omega}}\| < \infty$$

so $AE_{\bar{\Omega}}$ is H-smooth by Theorem XIII.25 and the remark following its statement.

(b) Since $(AR(\lambda + i\varepsilon)A^*)^* = AR(\lambda - i\varepsilon)A^*$,

$$c = \sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} \|AR(\lambda + i\varepsilon)A^*\| < \infty$$

Thus

$$\begin{aligned}
&\sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} |\varepsilon| \|R(\lambda + i\varepsilon)A^*\|^2 \\
&\quad = \sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} |\varepsilon| \|AR(\lambda + i\varepsilon)R(\lambda - i\varepsilon)A^*\| \\
&\quad = \sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} \tfrac{1}{2}\|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]A^*\| \leq c < \infty
\end{aligned}$$

Since $\|R(\lambda + i\varepsilon)A^*\| = \|AR(\lambda - i\varepsilon)\|$, the conditions of (a) hold. ∎

We can now state the extension of Theorem XIII.24.

Theorem XIII.31 Let H and H_0 be self-adjoint operators with spectral projections E_Ω and $E_\Omega^{(0)}$. Suppose that

$$H - H_0 = A^*B$$

in the sense of (35). Suppose that A is H-bounded and H-smooth on some bounded open interval $\Omega \subset \mathbb{R}$ and that B is H_0-bounded and H_0-smooth on Ω. Then the limits

$$W_\pm = \operatorname*{s-lim}_{t \to \mp\infty} e^{iHt} e^{-iH_0 t} E_\Omega^{(0)}$$

and

$$\tilde{W}_\pm = \operatorname*{s-lim}_{t \to \mp\infty} e^{iH_0 t} e^{-iHt} E_\Omega$$

exist. Moreover,

$$W_\pm^* = \tilde{W}_\pm \tag{52}$$

$$\tilde{W}_\pm W_\pm = E_\Omega^{(0)}; \qquad W_\pm \tilde{W}_\pm = E_\Omega \tag{53}$$

Proof Suppose that we prove that $W_\pm$ exist and that Ran $W_\pm \subset E_\Omega$. Then, by symmetry, and the fact that $H_0 - H = -B^*A$, $\tilde{W}_\pm$ exist and Ran $\tilde{W}_\pm \subset E_\Omega^{(0)}$. (52) is obvious, and (53) follows from the fact that $W_\pm$ (respectively $\tilde{W}_\pm$) is a partial isometry with initial space $E_\Omega^{(0)}$ (respectively E_Ω). We shall show that $W_\pm$ exist and Ran $W_\pm \subset E_\Omega$ by proving that s-lim$_{t \to \mp\infty} E_\Omega e^{iHt} e^{-iH_0 t} E_\Omega^{(0)}$ exists and

$$\operatorname*{s-lim}_{t \to \mp\infty} E_{\mathbb{R}\setminus\Omega} e^{iHt} e^{-iH_0 t} E_\Omega^{(0)} = 0 \tag{54}$$

The proof that the first limit exists is identical to the proof of Theorem XIII.24. It is obviously sufficient to prove (54) with $E_\Omega^{(0)}$ replaced by $E_I^{(0)}$ for an arbitrary compact subinterval $I \subset \Omega$. Given such an I, let C be the contour in Figure XIII.4. Then

$$\begin{aligned} &E_{\mathbb{R}\setminus\Omega} e^{iHt} e^{-iH_0 t} E_I^{(0)} \varphi \\ &\quad = \frac{1}{2\pi i} \oint_C E_{\mathbb{R}\setminus\Omega} (H - z)^{-1} e^{iHt} e^{-iH_0 t} E_I^{(0)} \varphi \, dz \\ &\quad - \frac{1}{2\pi i} \oint_C E_{\mathbb{R}\setminus\Omega} e^{iHt} e^{-iH_0 t} (H_0 - z)^{-1} E_I^{(0)} \varphi \, dz \\ &\quad = \frac{1}{2\pi i} \oint_C E_{\mathbb{R}\setminus\Omega} e^{iHt} [(H - z)^{-1} - (H_0 - z)^{-1}] e^{-iH_0 t} E_I^{(0)} \varphi \, dz \end{aligned}$$

Since this last integrand is uniformly bounded on C, it is sufficient, by the dominated convergence theorem, to prove that

$$\operatorname*{s-lim}_{t \to \mp\infty} [(H - z)^{-1} - (H_0 - z)^{-1}] e^{-iH_0 t} E_I^{(0)} = 0 \tag{55}$$

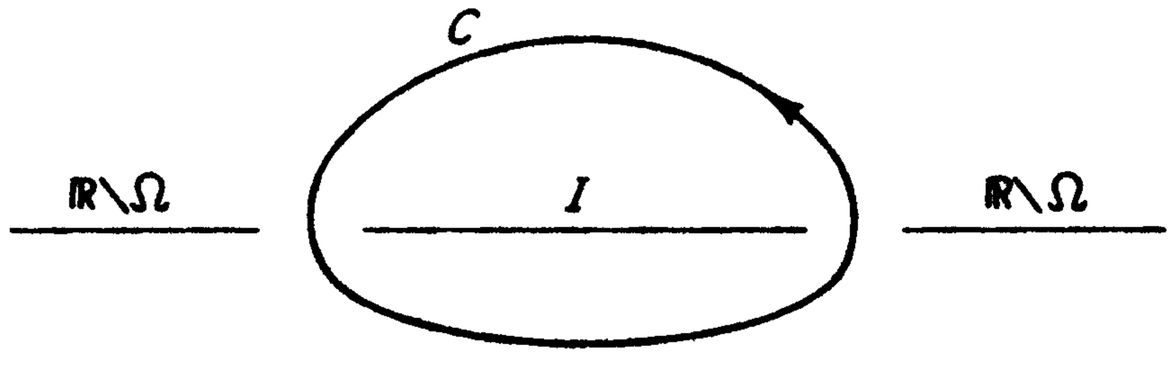


FIGURE XIII.4 A contour of integration.

for all nonreal z. But

$$\begin{aligned} &|(\psi, [(H-z)^{-1} - (H_0 - z)^{-1}]e^{-iH_0 t}E_I^{(0)}\varphi)| \\ &\quad = |(A(H-z)^{-1}\psi, B(H_0 - z)^{-1}e^{-iH_0 t}E_I^{(0)}\varphi)| \\ &\quad \leq \|A(H-z)^{-1}\| \, \|B(H_0 - z)^{-1}e^{-iH_0 t}E_I^{(0)}\varphi\| \, \|\psi\| \end{aligned}$$

Thus, to prove (55) we need only show

$$\lim_{t \to \pm\infty} \|B(H_0 - z)^{-1}e^{-iH_0 t}E_I^{(0)}\varphi\| = 0 \tag{56}$$

But, by the smoothness hypothesis, the function of t in (56) is square-integrable. Moreover, it has a uniformly bounded derivative, so (56) holds (Problem 62). ∎

Corollary Suppose that H and H_0 are self-adjoint with spectral projections E_Ω and $E_\Omega^{(0)}$ and that

$$H - H_0 = A^*B$$

where B is H_0-bounded and A is H-bounded. Let $S \subset \mathbb{R}$ with $S = \bigcup_{i=1}^{\infty} \Omega_i$ and each Ω_i a bounded open interval. Suppose that:

(i) A is H-smooth on each Ω_i and B is H_0-smooth on each Ω_i.
(ii) Both $\sigma(H)\backslash S$ and $\sigma(H_0)\backslash S$ have Lebesgue measure zero.

Then the generalized wave operators $\text{s-lim}_{t \to \mp\infty} e^{iHt}e^{-iH_0 t}E_{\text{ac}}^{(0)}$ exist and are complete.

Proof Since $S = \bigcup_{i=1}^{\infty} \Omega_i$ and $E_{\text{ac}}^{(0)} = E_S^{(0)}$, existence follows if we can prove that $\lim_{t \to \mp\infty} e^{iHt}e^{-iH_0 t}\varphi$ exists for $\varphi \in \bigcup_{i=1}^{\infty} \text{Ran } E_{\Omega_i}^{(0)}$. This is a direct consequence of the theorem. Since the inverse wave operators exist by symmetry, the wave operators are complete. ∎

One application of this corollary will be given in Section 8. Here we apply it to prove a result in the theory of repulsive potentials. This result is not the best possible (see the Notes).

Theorem XIII.32 Let H be an operator of the form given in the corollary of Theorem XIII.29. Suppose that each V_{ij} is a function of $|x|$ obeying $|V_{ij}(x)| \leq C(1 + |x|)^{-\frac{1}{2}-\varepsilon}$ for each i and j and some $\varepsilon > 0$. Then the wave operators $\Omega^{\pm} = \text{s-lim}_{t \to \mp\infty} e^{iHt}e^{-iH_0t}$ exist and are unitary.

Proof Since we already know that H has purely absolutely continuous spectrum, it is sufficient to prove that the wave operators exist and are complete. In the notation used in the proof of Theorem XIII.29, let

$$A_{jk} = +i\left[g(r_j - r_k)\frac{d}{dr_{jk}} + \frac{d}{dr_{jk}}g(r_j - r_k)\right], \qquad A = \sum_{j=k} A_{jk}$$

where $r_{jk} = |r_j - r_k|$ and d/dr_{jk} is defined by

$$r_{jk}\frac{d}{dr_{jk}} = (r_j - r_k)\cdot(\nabla_j - \nabla_k)$$

Now, $i[A_{ij}, V_{ij}] \geq 0$ as in the proof of Theorem XIII.29 and $i[A_{k\ell}, V_{ij}] = 0$ for i, j, k, ℓ distinct. Finally, for i, j, k distinct,

$$i[A_{ik} + A_{kj}, V_{ij}(r_{ij})] = \mathbf{a}(i, j, k)\cdot(\nabla V_{ij})(r_{ij})$$

where $\mathbf{a}(i, j, k) = g(r_{ik})\mathbf{e}_{ik} + g(r_{kj})\mathbf{e}_{kj}$ and $\mathbf{e}_{ik} = r_{ik}^{-1}(\mathbf{r}_i - \mathbf{r}_k)$. Since V_{ij} is only a function of $|x|$ and $(\mathbf{x}\cdot\nabla)V_{ij} \leq 0$, we can conclude that $i[A_{ik} + A_{kj}, V_{ij}] \geq 0$ if $(\mathbf{r}_i - \mathbf{r}_j)\cdot(\mathbf{a}(i, j, k)) \geq 0$. But

$$\begin{aligned}(\mathbf{r}_i - \mathbf{r}_j)\cdot\mathbf{a}(i, j, k) &= r_{ik}g(r_{ik}) + r_{kj}g(r_{kj}) \\ &\quad + (e_{ik}\cdot e_{kj})(r_{ik}g(r_{kj}) + r_{kj}g(r_{ik})) \\ &\geq (r_{ik} - r_{kj})(g(r_{ik}) - g(r_{jk})) \\ &\geq 0\end{aligned}$$

since g is monotone. It follows that $i[A, V] \geq 0$ so that computations identical to those used in Theorem XIII.29 show that (Problem 64):

$$i[A, H] \geq c(1 + r_{jk})^{-3-\varepsilon}$$

for a suitable constant c. Again, following the proof of Theorem XIII.29, we conclude that $(1 + r_{jk})^{-\frac{1}{2}-\varepsilon}(H + I)^{-1}$ is H-smooth. Since

$$\| |V_{ij}|^{3/5}(H + I)^{-1}e^{-iHt}\varphi\| \leq c^{1/2}\|(1 + r_{jk})^{-\frac{1}{2}-\varepsilon}(H + I)^{-1}e^{-iHt}\varphi\|$$

$|V_{ij}|^{3/5}(H + I)^{-1}$ is H-smooth and thus $|V_{ij}|^{3/5}$ is H-smooth on any compact set. By hypothesis, $|V_{ij}|^{2/5} \in L^{m+\varepsilon}(\mathbb{R}^m) \cap L^{m-\varepsilon}(\mathbb{R}^m)$, so by the proof of Theorem XIII.27, $|V_{ij}|^{2/5}$ is H_0-smooth. The result now follows from the previous corollary. ∎

XIII.8 The absence of singular continuous spectrum III: Weighted L^2 spaces

We have seen that a sufficient condition for $\sigma_{\text{sing}}(H)$ to be empty is that there be a dense set of vectors $X \subset \mathscr{H}$ so that $(\varphi, (H - z)^{-1}\varphi)$ remains bounded as $z \to \lambda \in \mathbb{R}$ for any $\varphi \in X$. There is a natural way of approaching this condition. Suppose that $X \subset \mathscr{H}$ is dense and that there is a norm $|||\cdot|||_+$ on X so that X is a Banach space and so that $|||\varphi|||_+ \geq \|\varphi\|$ for any $\varphi \in X$. Then the inner product on $\mathscr{H}$ allows one to realize $\mathscr{H}$ in a natural way as a subset of X^*. If $|||\cdot|||_-$ denotes the norm on X^*, then $\|\varphi\| \geq |||\varphi|||_-$ for any $\varphi \in \mathscr{H}$. We have already discussed such a situation and related ideas in Section VIII.6 and the appendix to Section XI.6. Let $z \in \mathbb{C}$ with $\operatorname{Im} z \neq 0$. Then $(H - z)^{-1}$ takes $\mathscr{H}$ into $\mathscr{H}$ and so X into X^*. Of course the norm of $(H - z)^{-1}$ as a map from $\mathscr{H}$ to $\mathscr{H}$ diverges as z approaches $\sigma(H)$, but suppose that it remains bounded as a map of X into X^*. Then

$$|(\varphi, (H - z)^{-1}\varphi)| \leq |||\varphi|||_+^2 \, \|(H - z)^{-1}\|_{+,-}$$

where

$$\|A\|_{+,-} = \sup_{\psi \neq 0, \psi \in X} \|A\psi\|_- / \|\psi\|_+$$

so we can conclude that $\sigma_{\text{sing}}(H) = \varnothing$, by Theorem XIII.20.

It is natural to try to implement this idea with perturbation techniques. That is, we consider $H = H_0 + V$ and begin by proving bounds on $(H_0 - z)^{-1}$ as a map from X to X^*. We shall consider Schrödinger operators and take $H_0 = -\Delta$. To motivate our choice of X, let $f \in \mathscr{S}(\mathbb{R}^n)$ and consider

$$\begin{aligned}
&\lim_{y \downarrow 0} (f, [(H_0 - x + iy)^{-1} - (H_0 - x - iy)^{-1}]f) \\
&\quad = \lim_{y \downarrow 0} \int |\hat{f}(p)|^2 2i \operatorname{Im}[(p^2 - x + iy)^{-1}] \, d^n p \\
&\quad = -2i\pi \int |\hat{f}(p)|^2 \, \delta(p^2 - x) \, d^n p
\end{aligned}$$

by Eq. (V.4). Thus, for $(f, (H_0 - x + iy)^{-1}f)$ to have a limit as $y \downarrow 0$, $\hat{f}$ must have a "natural" restriction to the sphere of radius $x^{1/2}$. Because of our discussion in Section IX.9, it is natural to choose X as an L^2_δ space (with $\delta > \frac{1}{2}$) so that X^* is $L^2_{-\delta}$:

$$L^2_\delta(\mathbb{R}^n) = \left\{ f(x) \,\middle|\, \|f\|_\delta^2 \equiv \int (1 + x^2)^\delta |f(x)|^2 \, dx < \infty \right\}$$

We shall lean heavily on the estimates proven in Section IX.9, especially Theorems IX.39 and IX.41.

Definition A multiplication operator is called an **Agmon potential** if $V(x) = (1 + x^2)^{-\frac{1}{4}-\varepsilon}W(x)$ for some $\varepsilon > 0$ and some W that is a relatively compact perturbation of $-\Delta$.

The Agmon potentials form a vector space of $-\Delta$-bounded perturbations of relative bound zero (see Problem 20 of Chapter X).

Example 1 Let $p > n/2$, $p < \infty$, and $p \geq 2$. Then any $W \in L^p(\mathbb{R}^n)$ is relatively compact (Problem 41), so any V with $(1 + x^2)^{\frac{1}{4}+\varepsilon}V \in L^p$ is an Agmon potential.

Example 2 Let $W \in L^\infty(\mathbb{R}^n)$ and define $V(x) = (1 + x^2)^{-\frac{1}{4}-\varepsilon}W(x)$. To show that V is an Agmon potential we need only prove that $U(x) = (1 + x^2)^{-\varepsilon/2}W(x)$ is relatively compact. But this is true since $U(x)$ is in $L^p + (L^\infty)_\varepsilon$ for all p (Problem 41).

The main theorem of this section is:

Theorem XIII.33 (the Agmon–Kato–Kuroda theorem) Let V be an Agmon potential and let $H = H_0 + V$ where $H_0 = -\Delta$. Then:

(a) The set $\mathscr{E}_+$ of positive eigenvalues of H is a discrete subset of $(0, \infty)$, and each eigenvalue has finite multiplicity.
(b) If C is any compact subinterval of $(0, \infty)\backslash\mathscr{E}_+$ and if $\delta > \frac{1}{2}$, then

$$\sup_{\lambda \in C,\, 0<y<1} \sup_{\psi,\, \varphi \in L^2_\delta;\, \|\varphi\|_\delta \leq 1,\, \|\psi\|_\delta \leq 1} |(\psi, (H - \lambda - iy)^{-1}\varphi)| < \infty$$

(c) $\sigma_{\text{sing}}(H) = \varnothing$.
(d) The wave operators $\Omega^\pm(H, H_0)$ exist and are complete.

The proof of Theorem XIII.33, while elegant, is rather long so we break it up into a series of lemmas. After proving (a), we develop a few technical estimates that will allow us to prove (c) and (d) from (b); then we prove (b) in case $V = 0$; finally, we use the estimates proven for H_0, Theorem IX.39, Theorem IX.41, and a bootstrap argument to complete the proof. Throughout we let $\rho(x) \equiv (1 + x^2)^{1/2}$. The use of the weighted L^2 spaces and Theorem IX.39 is illustrated in:

Proof of (a) of Theorem XIII.33 Suppose that $\varphi \in D(H)$ and $H\varphi = \lambda\varphi$ with $\lambda > 0$. First, we shall show that $\|\varphi\|_\delta \leq c\|\varphi\|$ for some $\delta > 0$ where c depends only on λ and remains bounded as λ varies through compact subsets of

$(0, \infty)$. Since W is H_0-compact, it is H-bounded so that $\|W\varphi\| \leq a\|H\varphi\| + b\|\varphi\| = (a\lambda + b)\|\varphi\|$. As a result $\psi \equiv V\varphi = \rho^{-1-\varepsilon}W\varphi$ is in $L^2_{1+\varepsilon}$. In particular, by Theorem IX.40, $\hat{\psi}$ has restrictions to each sphere S_E, and the restriction is Hölder continuous in E. Since $(H_0 - \lambda)\varphi = -\psi$, $\hat{\varphi} = -(k^2 - \lambda)^{-1}\hat{\psi}$. If $\hat{\psi} \restriction S_{\sqrt{\lambda}}$ were not identically zero, then $\hat{\varphi}$ could not be in L^2, so we conclude that $\hat{\psi} \restriction S_{\sqrt{\lambda}} = 0$. As a result, Theorem IX.41 is applicable, so

$$\|\varphi\|_{\varepsilon/2} \leq c_\lambda \|\psi\|_{1+\varepsilon} = c_\lambda \|W\varphi\| \leq d_\lambda \|\varphi\|$$

Let $\eta \equiv \rho^{\varepsilon/2}(-\Delta + 1)\varphi$. Then $H\varphi = \lambda\varphi$ implies that

$$\begin{aligned}\|\eta\| &\leq \|\rho^{\varepsilon/2}(\lambda + 1)\varphi\| + \|\rho^{\varepsilon/2}V\varphi\| \\ &\leq (\lambda + 1)\|\varphi\|_{\varepsilon/2} + \|W\varphi\| \leq c'_\lambda \|\varphi\|\end{aligned}$$

Since $\varphi = (-\Delta + 1)^{-1}\rho^{-\varepsilon}\eta$, we conclude that for any compact subset K in $(0, \infty)$, any solution of $H\varphi = \lambda\varphi$ with $\lambda \in K$ and $\|\varphi\| = 1$ is of the form $\varphi = A\eta$ where: (i) $A = (-\Delta + 1)^{-1}\rho^{-\varepsilon}$ and (ii) $\|\eta\| \leq c$, a constant only depending on K. By Problem 41, A is a compact operator, so the set $M = \{\varphi = A\eta \mid \|\eta\| \leq c\}$ is compact. If any eigenvalue $\lambda \in K$ were of infinite multiplicity or if there were infinitely many eigenvalues in K, M would contain an infinite orthonormal set. Since M is compact, K contains only finitely many eigenvalues and each is of finite multiplicity. ∎

We note that we shall show that $\mathscr{E}_+ = \varnothing$ under some additional regularity hypotheses on V in Section 13.

Lemma 1 Let F and G be any two real-valued multiplication operators that are H_0-bounded with relative bound zero. Then for any $\mu \in \mathbb{C}\backslash\mathbb{R}$, $(H_0 - \mu)^{-1}$, $(H_0 + G - \mu)^{-1}$, $F(H_0 - \mu)^{-1}$, and $F(H_0 + G - \mu)^{-1}$ are bounded on each L^2_δ. Moreover, if F is also H_0-relatively compact, then $F(H_0 - \mu)^{-1}$ and $F(H_0 + G - \mu)^{-1}$ are compact on each L^2_δ.

Proof We shall prove the lemma for $(H_0 - \mu)^{-1}$ in the case $|\delta| \leq 1$. The other cases are similar and are left to the problems (Problem 66). Introduce the symbol ∂_j for the operator $\partial/\partial x_j$ and consider the formal computation

$$\begin{aligned}[(H_0 - \mu)^{-1}, \rho^\delta] &= -(H_0 - \mu)^{-1}[H_0, \rho^\delta](H_0 - \mu)^{-1} \\ &= \sum_{i=1}^{n} \{(H_0 - \mu)^{-1}\,\partial_i\}(\partial_i \rho^\delta)(H_0 - \mu)^{-1} \\ &\quad + (H_0 - \mu)^{-1}(\partial_i \rho^\delta)\{\partial_i (H_0 - \mu)^{-1}\}\end{aligned}$$

Applied to vectors in $\mathscr{S}$, all computations are legitimate. Moreover, if $\delta \leq 1$, $\partial_i(\rho^\delta)$ is bounded. Since $(H_0 - \mu)^{-1}$ and $\partial_i(H_0 - \mu)^{-1}$ are bounded on L^2 we conclude that

$$\|[(H_0 - \mu)^{-1}, \rho^\delta]\psi\| \leq \text{const}\|\psi\|$$

if ψ is in $\mathscr{S}$ and so for arbitrary ψ in L^2. Suppose $1 \geq \delta > 0$. Then

$$\begin{aligned}\|(H_0 - \mu)^{-1}\psi\|_\delta &= \|\rho^\delta(H_0 - \mu)^{-1}\psi\| \\ &\leq \|(H_0 - \mu)^{-1}\| \, \|\psi\|_\delta + \|[(H_0 - \mu)^{-1}, \rho^\delta]\psi\| \\ &\leq d\|\psi\|_\delta\end{aligned}$$

so $(H_0 - \mu)^{-1}$ is bounded from L^2_δ to L^2_δ. By duality, $(H_0 - \bar{\mu})^{-1}$ is bounded from $L^2_{-\delta}$ to $L^2_{-\delta}$. ∎

Lemma 2 Let $H = H_0 + V$ as in Theorem XIII.33. Suppose that F is an Agmon potential and that for some compact interval $\Omega \subset \mathbb{R}$, and each $\delta > \frac{1}{2}$,

$$\sup_{x \in \Omega,\, 0<y<1} \; \sup_{\psi,\, \varphi \in L^2_\delta;\, \|\varphi\|_\delta \leq 1,\, \|\psi\|_\delta \leq 1} |(\psi, (H - \lambda - iy)^{-1}\varphi)| < \infty \tag{57}$$

Then $|F|^{1/2}$ is H-smooth on Ω.

Proof By Theorem XIII.30, we need only prove that

$$\sup_{\substack{\lambda \in \Omega \\ 0<y<1}} \| \, |F|^{1/2}(H - \lambda - iy)^{-1} \, |F|^{1/2}\| < \infty$$

(57) implies that $(H - \lambda - iy)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ for $\lambda + iy \in \Omega \times (0, 1)$. Write $F = \rho^{-1-\varepsilon}G$ where G is H_0-compact and let $\delta = \frac{1}{2} + (\varepsilon/2)$. Then, by Lemma 1, $(H - i)^{-1}|G|^{1/2}$ is bounded from L^2_δ to L^2_δ so $|G|^{1/2}(H - i)^{-1}(H - \lambda - iy)^{-1}(H - i)^{-1}|G|^{1/2}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ for $\lambda + iy \in \Omega \times (0, 1)$. Thus

$$|F|^{1/2}(H - i)^{-1}(H - \lambda - iy)^{-1}(H - i)^{-1}|F|^{1/2}$$

is uniformly bounded from L^2 to L^2 for $\lambda + iy \in \Omega \times (0, 1)$. Writing

$$\begin{aligned}(H - z)^{-1} = (H - i)^{-1} &+ (z - i)(H - i)^{-2} \\ &+ (z - i)^2(H - i)^{-1}(H - z)^{-1}(H - i)^{-1}\end{aligned}$$

and using the fact that $\| \, |F|^{1/2}(H - i)^{-1} \, |F|^{1/2}\| < \infty$, we see that

$$\sup_{\lambda + iy \in \Omega \times (0,\, 1)} \| \, |F|^{1/2}(H - \lambda - iy)^{-1} \, |F|^{1/2}\| < \infty. \; ∎$$

Reduction of Theorem XIII.33 to the proof of (*b*) We want to show that once we prove (b), then (c) and (d) follow. Suppose that (b) holds, that $\varphi \in L^2_\delta$ for $\delta > \frac{1}{2}$, and that K is a compact subinterval of $(0, \infty)\backslash\mathscr{E}_+$. Then $E_K\varphi \in \mathscr{H}_{ac}$ by Theorem XIII.20. Thus $K \cap \sigma_{sing} = \varnothing$. By the second corollary to Theorem XIII.14, $\sigma_{ess} = [0, \infty)$, so we conclude that $\sigma_{sing} \cap (-\infty, 0) = \varnothing$. Therefore, $\sigma_{sing} \subset (\mathscr{E}_+ \cup \{0\})$. $\mathscr{E}_+$ is countable by (a), so $\sigma_{sing} = \varnothing$. Applying Lemma 2 to the case $V = 0$, we see that $|V|^{1/2}$ is H_0-smooth on Ω for any interval $[a, b]$ with $a > 0$. In addition, $|V|^{1/2}$ is H-smooth on any such Ω with $\Omega \cap \mathscr{E}_+ = \varnothing$. (d) now follows from the corollary of Theorem XIII.31. ∎

The remainder of this section is devoted to proving (b). We first prove the case $V = 0$, which is an estimate quite similar to Theorem IX.41. The proof is also quite similar.

Lemma 3 Let $\varepsilon > 0$. Then there exists a constant c so that for all $\lambda \in \mathbb{C}$ and all $\varphi \in \mathscr{S}(\mathbb{R})$

$$\|\varphi\|_{-\frac{1}{2}-\varepsilon} \leq c\left\|\left(\frac{d}{dx} - \lambda\right)\varphi\right\|_{\frac{1}{2}+\varepsilon} \tag{58}$$

Proof Suppose that $\operatorname{Re}\lambda \leq 0$. Let $\psi = (d/dx - \lambda)\varphi$. Then

$$\varphi(x) = \int_{-\infty}^{x} e^{\lambda(x-y)}\psi(y)\,dy$$

Thus

$$\begin{aligned}\|\varphi\|_{L^\infty} \leq \|\psi\|_{L^1} &= ((1 + x^2)^{-\frac{1}{2}-\frac{1}{2}\varepsilon}, (1 + x^2)^{\frac{1}{2}+\frac{1}{2}\varepsilon}\psi) \\ &\leq c_1\|\psi\|_{\frac{1}{2}+\varepsilon}\end{aligned}$$

Since

$$\|\varphi\|_{-\frac{1}{2}-\varepsilon} \leq \|\varphi\|_{L^\infty}\|(1 + x^2)^{-\frac{1}{2}-\frac{1}{2}\varepsilon}\|_{L^2}$$

(58) follows in the case $\operatorname{Re}\lambda \leq 0$. A similar argument works for $\operatorname{Re}\lambda \geq 0$. ∎

Lemma 4 Let n be fixed. Then for all $\varepsilon > 0$, there is a constant d so that for all $\lambda \in \mathbb{C}$, each $j = 1, \ldots, n$, and all $\varphi \in \mathscr{S}(\mathbb{R}^n)$,

$$\|\partial_j\varphi\|_{-\frac{1}{2}-\varepsilon} \leq d\|(-\Delta - \lambda)\varphi\|_{\frac{1}{2}+\varepsilon} \tag{59}$$

Proof Consider first the case $n = 1$. Let $\lambda = -\mu^2$. Then by Lemma 3,

$$\left\| \frac{d}{dx}\varphi \right\|_{-\frac{1}{2}-\varepsilon} \leq \frac{1}{2}\left\| \left(\frac{d}{dx} - \mu\right)\varphi \right\|_{-\frac{1}{2}-\varepsilon} + \frac{1}{2}\left\| \left(\frac{d}{dx} + \mu\right)\varphi \right\|_{-\frac{1}{2}-\varepsilon}$$

$$\leq c\left\| \left(-\frac{d^2}{dx^2} - \lambda\right)\varphi \right\|_{\frac{1}{2}+\varepsilon}$$

Now let $\varphi \in \mathscr{S}(\mathbb{R}^n)$ and let $\psi(x_1, k_2, \ldots, k_n)$ be the partial Fourier transform of φ with respect to $x_2, \ldots, x_n$,

$$\psi(x_1, k_2, \ldots, k_n) = (2\pi)^{-(n-1)/2} \int e^{-i\sum_2^n k_j x_j}\varphi(x_1, \ldots, x_n)\, dx_2 \cdots dx_n$$

Using the one-dimensional result, for each fixed $k_2, \ldots, k_n$,

$$\int (1 + x_1^2)^{-\frac{1}{2}-\varepsilon} |\partial_1 \psi(x_1, k_2, \ldots, k_n)|^2\, dx_1$$

$$\leq c \int (1 + x_1^2)^{\frac{1}{2}+\varepsilon} |(-\partial_1^2 + k_2^2 + \cdots + k_n^2 - \lambda)\psi|^2\, dx_1$$

Integrating with respect to $k_2, \ldots, k_n$ and using the Plancherel theorem, we see that

$$\int (1 + x_1^2)^{-\frac{1}{2}-\varepsilon} |\partial_1 \varphi(x)|^2\, d^n x \leq c \int (1 + x_1^2)^{\frac{1}{2}+\varepsilon} |(-\Delta - \lambda)\varphi|^2\, d^n x$$

Since $(1 + x^2)^{-\frac{1}{2}-\varepsilon} \leq (1 + x_1^2)^{-\frac{1}{2}-\varepsilon}$ and $(1 + x_1^2)^{\frac{1}{2}+\varepsilon} \leq (1 + x^2)^{\frac{1}{2}+\varepsilon}$, (59) follows. ∎

Lemma 5 Let n be fixed. For any compact set $K \subset \mathbb{C}\backslash\{0\}$, there is a constant c so that for all $\lambda \in K$ and $\varphi \in \mathscr{S}(\mathbb{R}^n)$,

$$\|\varphi\|_{-\frac{1}{2}-\varepsilon} \leq c\|(-\Delta - \lambda)\varphi\|_{\frac{1}{2}+\varepsilon} \tag{60}$$

Proof We can find $c_1 > 0$ satisfying

$$\inf_{x \in \mathbb{R},\, \lambda \in K} [|x^2 - \lambda|^2 + |x|^2] \geq c_1^{-2}$$

Therefore, given $\psi \in \mathscr{S}(\mathbb{R}^n)$

$$|\hat{\psi}(k_1, \ldots, k_n)|^2 \leq c_1^2 \left[|(\textstyle\sum k_i^2 - \lambda)\hat{\psi}(k_1, \ldots, k_n)|^2 + \sum_{i=1}^n |k_i \hat{\psi}(k_1, \ldots, k_n)|^2 \right]$$

Integrating and using the Plancherel theorem

$$\|\psi\|^2 \leq c_1^2 \left[\|(-\Delta - \lambda)\psi\|^2 + \sum_{j=1}^n \|\partial_j \psi\|^2 \right] \tag{61a}$$

for all $\lambda \in K$. Let α be a positive real number which we shall adjust below. Set $\delta = \frac{1}{2} + \varepsilon$ and $\rho_\alpha = (1 + \alpha x^2)^{1/2}$. Finally, let $\varphi = (\rho_\alpha)^\delta \psi$. Then, by (61a)

$$\|\rho_\alpha^{-\delta}\varphi\| \leq c_1 \|(-\Delta - \lambda)\rho_\alpha^{-\delta}\varphi\| + c_1 \sum_{j=1}^{n} \|\partial_j \rho_\alpha^{-\delta}\varphi\| \tag{61b}$$

Now $\partial_j \rho_\alpha^{-\delta}\varphi = \rho_\alpha^{-\delta}\, \partial_j \psi - \delta\alpha x_j \rho_\alpha^{-\delta-1}\varphi$ so

$$\|\partial_j \rho_\alpha^{-\delta}\varphi\| \leq \|\rho_\alpha^{-\delta}\, \partial_j \varphi\| + \alpha^{1/2}\, \delta \|\rho_\alpha^{-\delta}\varphi\|$$

since $|\alpha^{1/2} x_j \rho^{-1}| \leq 1$ for all x. Similarly (Problem 67),

$$\|(-\Delta - \lambda)\rho_\alpha^{-\delta}\varphi\| \leq \|\rho_\alpha^{-\delta}(-\Delta - \lambda)\varphi\| + 2\, \delta\alpha^{1/2} \sum_{j=1}^{n} \|\rho_\alpha^{-\delta}\, \partial_j \varphi\|$$

$$+ d_{n,\varepsilon}\alpha \|\rho_\alpha^{-\delta}\varphi\| \tag{62}$$

where $d_{n,\varepsilon}$ is only dependent on ε and n. Pick α so small that $c_1(n\, \delta\alpha^{1/2} + d_{n,\varepsilon}\alpha) < \frac{1}{2}$ and $\alpha < 1$. Then, by (61), for all $\varphi \in \mathscr{S}$ and $\lambda \in K$,

$$\tfrac{1}{2}\|\rho_\alpha^{-\delta}\varphi\| \leq c_2 \left| \|\rho_\alpha^{-\delta}(-\Delta - \lambda)\varphi\| + \sum_{j=1}^{n} \|\rho_\alpha^{-\delta}\, \partial_j \varphi\| \right|$$

Since $\rho^{-\delta} \leq \rho_\alpha^{-\delta} \leq \alpha^{-\delta/2}\rho^{-\delta}$, we have that

$$\|\varphi\|_{-\delta} \leq c_3[\|(-\Delta - \lambda)\varphi\|_{-\delta} + \sum_j \|\partial_j \varphi\|_{-\delta}]$$

where c_3 is independent of $\lambda \in K$ and $\varphi \in \mathscr{S}$. Since $\|\cdot\|_{-\delta} \leq \|\cdot\|_\delta$ and $\|\partial_j \varphi\|_{-\delta} \leq c\|(-\Delta - \lambda)\varphi\|_\delta$ by Lemma 4, (60) follows. ∎

If now $\operatorname{Im} \lambda \neq 0$ and $\delta > \frac{1}{2}$, then by Lemma 1, $(H_0 - \lambda)^{-1}$ is a bounded map from L^2_δ to L^2_δ. Lemma 5 assures us that, for $\lambda \in K = [a, b] \times (0, 1]$ $(a > 0)$, we have the basic estimate

$$\|(H_0 - \lambda)^{-1}\varphi\|_{-\delta} \leq c\|\varphi\|_\delta \tag{63}$$

Given (63), it is natural to consider the boundary values $\lim_{y \downarrow 0} (H_0 - x - iy)^{-1}$ as maps of L^2_δ to $L^2_{-\delta}$. Such boundary values are not strictly necessary for the proof, but they help to make it more conceptual, so we introduce them. As preparation, we need

Lemma 6 Let $\delta > \frac{3}{2}$ and let $0 < a < b$. Then there is a constant c so that for all $\varphi \in L^2_\delta$ and $\lambda = x + iy$ with $x \in [a, b]$ and $y \in (0, 1]$,

$$\|(H_0 - \lambda)^{-2}\varphi\|_{-\delta} \leq c\|\varphi\|_\delta$$

Proof Let A be the operator $\sum_{j=1}^{n} x_j \partial_j$. Then $[A, (H_0 - \lambda)] = -2H_0$ so that

$$\begin{aligned}[A, (H_0 - \lambda)^{-1}] &= -(H_0 - \lambda)^{-1}[A, (H_0 - \lambda)](H_0 - \lambda)^{-1} \\ &= 2H_0(H_0 - \lambda)^{-2} \\ &= 2(H_0 - \lambda)^{-1} + 2\lambda(H_0 - \lambda)^{-2}\end{aligned}$$

where all the computations are legitimate when applied to vectors in $\mathscr{S}(\mathbb{R}^n)$. Since $(H_0 - \lambda)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$, we need only prove that $[A, (H_0 - \lambda)^{-1}]$ is bounded from L^2_δ to $L^2_{-\delta}$, uniformly for λ satisfying $a \leq \operatorname{Re} \lambda \leq b$, $0 < \operatorname{Im} \lambda \leq 1$. It is thus sufficient to prove that $\rho^{-\delta}(x_j \partial_j) \times (H_0 - \lambda)^{-1}\rho^{-\delta}$ is bounded on L^2 uniformly in λ. Write

$$(H_0 - \lambda)^{-1} = (H_0 + 1)^{-1} + (\lambda + 1)(H_0 + 1)^{-1}(H_0 - \lambda)^{-1}$$

Certainly $(\rho^{-\delta}x_j)[\partial_j(H_0 + 1)^{-1}]\rho^{-\delta}$ is bounded on L^2. Moreover

$$\rho^{-1}x_j[\rho^{-\delta+1}(\partial_j(H_0 + 1)^{-1})\rho^{\delta-1}](\rho^{-\delta+1}(H_0 - \lambda)^{-1}\rho^{-\delta+1})\rho^{-1}$$

is bounded for the first and last factor are trivially bounded, the third is bounded by Lemma 5, and the second is bounded by mimicking the proof of Lemma 1 (Problem 66c). ∎

Lemma 7 Let $\delta > \frac{1}{2}$ and let $x > 0$. Then $(H_0 - x - i0)^{-1} \equiv \lim_{y \downarrow 0} (H_0 - x - iy)^{-1}$ exists in norm as a map from L^2_δ to $L^2_{-\delta}$. Moreover:

(a) $V(H_0 - x - i0)^{-1}$ is compact as a map of L^2_δ to L^2_δ if V is an Agmon potential such that $\rho^{2\delta}V = W$ is relatively H_0-compact.

(b) $\operatorname{Im}(\varphi, (H_0 - x - i0)^{-1}\varphi) = (\pi/2)x^{\frac{1}{2}n-1} \int_{S^{n-1}} |\hat{\varphi}(x^{1/2}\Omega)|^2 \, d\Omega$ where $\hat{\varphi} \restriction S_{x^{1/2}}$ is defined by Theorem IX.39, and $d\Omega$ is the usual surface measure on the sphere.

Proof Let $\delta' = \delta + 1$. Then as operators from $L^2_{\delta'}$ to $L^2_{-\delta'}$

$$\begin{aligned}&\|(H_0 - \lambda_1)^{-1} - (H_0 - \lambda_2)^{-1}\| \\ &\quad \leq |\lambda_2 - \lambda_1| \sup_{0 \leq t \leq 1} \|[H_0 - t\lambda_1 - (1 - t)\lambda_2]^{-2}\|\end{aligned}$$

By Lemma 6, we see that $(H_0 - x - iy)^{-1}$ is norm Cauchy as $y \downarrow 0$. Let $\delta'' = \frac{1}{2}(\delta + \frac{1}{2})$. Then by Lemma 5, $(H_0 - x - iy)^{-1}$ is norm bounded as $y \downarrow 0$ as a map from $L^2_{\delta''}$ to $L^2_{-\delta''}$. Since $\delta'' < \delta < \delta'$, we can interpolate between the

δ' and δ'' results (see Example 3 of the appendix to Section IX.4) and conclude that as maps from L^2_δ to $L^2_{-\delta}$, $(H_0 - x - iy)^{-1}$ is norm Cauchy as $y \downarrow 0$. To prove (a) we write

$$W(H_0 - x - i0)^{-1} = W(H_0 + 1)^{-1} + (x + 1)W(H_0 + 1)^{-1}(H_0 - x - i0)^{-1}$$

and so conclude by Lemma 1 that $W(H_0 - x - i0)^{-1}$ is compact as a map from L^2_δ to $L^2_{-\delta}$. Since $\rho^{-2\delta}$ is an isometry from $L^2_{-\delta}$ to L^2_δ, (a) follows. Finally, (b) holds for $\varphi \in \mathscr{S}$ because of (V.4) (see Problem 22 of Chapter V). By Theorem IX.39, it extends to all $\varphi \in L^2_\delta$. ∎

Lemma 8 Let $\delta > \frac{1}{2}$ and let $\varphi \in L^2_\delta$ satisfy $\varphi = -V(H_0 - x - i0)^{-1}\varphi$ where $x > 0$, and V is an Agmon potential so that $\rho^{2\delta}V = W$ is relatively H_0-compact, and where $V(H_0 - x - i0)^{-1}$ is interpreted as the composition of maps $W(H_0 - x - i0)^{-1}$ from L^2_δ to $L^2_{-\delta}$ and $\rho^{-2\delta}$ from $L^2_{-\delta}$ to L^2_δ. Then:

(a) $\psi \equiv (H_0 - x - i0)^{-1}\varphi$ is in L^2.
(b) If $\varphi \neq 0$, then x is an eigenvalue of $H = H_0 + V$ as an operator on L^2.

Proof The argument is very similar to the proof of (a) of Theorem XIII.33. By the formula

$$(H_0 - x - i0)^{-1} = (H_0 + 1)^{-1} + (x + 1)(H_0 + 1)^{-1}(H_0 - x - i0)^{-1}$$

we see that $\psi \in (H_0 + 1)^{-1}[L^2_{-\delta}]$ so that $W\psi \in L^2_{-\delta}$ by Lemma 1. As a result, the integral $\int V(\xi)|\psi(\xi)|^2\, d\xi = (\rho^{-\delta}\psi, \rho^{-\delta}W\psi)$ is absolutely convergent and obviously real. But $V\psi = -\varphi$ so we conclude that $(\varphi, (H_0 - x - i0)^{-1}\varphi)$ is real. By Lemma 7, part (b), $\hat{\varphi} \restriction S_{x^{1/2}} \equiv 0$. As a result, Theorem IX.41 is applicable and we have the following "bootstrap" argument: Let $\delta = \frac{1}{2} + \varepsilon$. Since $\varphi \in L^2_\delta$, $\psi \in L^2_{\delta - 1 - \varepsilon}$ by Theorem IX.41. Using Lemma 1 and

$$W\psi = W(H_0 + 1)^{-1}\varphi + (x + 1)W(H_0 + 1)^{-1}\psi$$

we see that $W\psi \in L^2_{\delta - 1 - \varepsilon}$ also. Thus $\varphi = -V\psi = -\rho^{2\delta}W\psi$ is in $L^2_{\delta - 1 - \varepsilon + 2\delta} = L^2_{\delta + \varepsilon}$. By this argument we have improved the estimate $\varphi \in L^2_\delta$ to $\varphi \in L^2_{\delta + \varepsilon}$. There is nothing to stop us from repeating it! Thus, $\varphi \in L^2_{\delta + n\varepsilon}$ for all n so $\psi \in L^2_{\delta - 1 + (n-1)\varepsilon}$ for all n. In particular $\psi \in L^2$. For $\eta \in \mathscr{S}$,

$$(H_0\eta, \psi) = \lim_{y \downarrow 0} (\eta, H_0(H_0 - x - iy)^{-1}\varphi) = \lim_{y \downarrow 0} (\eta, (x + iy)\psi + \varphi)$$
$$= (\eta, x\psi + \varphi)$$

Therefore, $\psi \in D(H_0)$ and $H_0\psi = x\psi + \varphi = x\psi - V\psi$ so x is an eigenvalue of H as an operator on L^2. ∎

Completion of the proof of Theorem XIII.33 Choose $\delta > \frac{1}{2}$ so that $\rho^{2\delta}V = W$ is relatively H_0-compact. Given a compact subinterval $K \subset (0, \infty)\backslash\mathscr{E}_+$, consider the operator-valued function $A(\mu) = V(H_0 - \mu)^{-1}$ on $K \times [0, 1]$ where $(H_0 - \mu)^{-1}$ is interpreted as $(H_0 - x - i0)^{-1}$ if $\operatorname{Im} \mu = 0$. Then $A(\mu)$ is a function with values in the compact operators on L^2_δ, continuous on $K \times [0, 1]$ and analytic in its interior. Moreover, $A(\mu)\varphi = -\varphi$ has no nonzero solutions for $\mu \in K \times [0, 1]$. When $\operatorname{Im} \mu = 0$, this follows from the hypothesis $K \cap \mathscr{E}_+ = \varnothing$ and Lemma 8. For $\operatorname{Im} \mu \neq 0$, this follows from the facts that $(1 + V(H_0 - \mu)^{-1})(H_0 - \mu) = H - \mu$ and that both $H_0 - \mu$ and $H - \mu$ are invertible as maps of L^2_δ to L^2_δ by Lemma 1. It follows by a simple extension of the analytic Fredholm theorem (Theorem VI.14) that $(1 + A(\mu))^{-1}$ is a continuous function on $K \times [0, 1]$; in particular, it is uniformly bounded. But for $\operatorname{Im} \mu \neq 0$, $(H - \mu)^{-1} = (H_0 - \mu)^{-1} \times (1 + A(\mu))^{-1}$. Since $(H_0 - \mu)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ by Lemma 5 and $(1 + A(\mu))^{-1}$ is uniformly bounded from L^2_δ to L^2_δ, $(H - \mu)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ for $\mu \in K \times [0, 1]$. This is just a rephrasing of (b). ∎

XIII.9 The spectrum of tensor products

In Section VIII.10 we proved that if A and B are self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$ with domains D_1 and D_2, then $A \otimes I + I \otimes B$ is essentially self-adjoint on $D_1 \otimes D_2$ and $\sigma(A \otimes I + I \otimes B) = \sigma(A) + \sigma(B)$. The purpose of this section is to extend this result to the case where A and B are m-sectorial (see Section VIII.6). We shall exploit the connection between m-sectorial operators and bounded holomorphic semigroups (see Section X.8). In the self-adjoint case the proof was "easy" in the sense that it was a relatively straightforward consequence of the spectral theorem. In the m-sectorial case the use of the spectral theorem is replaced by the theory of commutative Banach algebras and the Laplace transform formulas relating bounded holomorphic semigroups to the resolvents of their generators. The reader is referred to the Notes for references about commutative Banach algebras. This section is divided into two parts. In the first part we prove that $\sigma(A \otimes B) = \sigma(A) \otimes \sigma(B)$ if A and B are bounded operators on $\mathscr{H}_1$ and $\mathscr{H}_2$. In the second part we apply this result to $e^{-tA} \otimes e^{-tB}$ where A and B are the generators of bounded holomorphic semigroups in order to obtain the desired result for m-sectorial operators.

Let A be a bounded operator on a Hilbert space $\mathscr{H}$. We shall denote by $\mathscr{R}(A)$ the Banach algebra of operators generated by the identity

and all the resolvents of A, i.e., $\mathscr{R}(A)$ is just the closure in the operator norm of the family of polynomials in finitely many variables in the resolvents of A at different points. $\mathscr{R}(A)$ is a commutative Banach algebra that contains A since $\lambda^2(\lambda - A)^{-1} - \lambda I \to A$ in norm as $\lambda \to \infty$. Since all the resolvents of A are in $\mathscr{R}(A)$ we have $\sigma(A) = \sigma_{\mathscr{R}(A)}(A)$ where $\sigma_{\mathscr{R}(A)}(A)$ denotes the Gel'fand spectrum of A with respect to $\mathscr{R}(A)$.

Let $\mathscr{R}(A)$ and $\mathscr{R}(B)$ be the resolvent algebras of A and B on $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively. Then if $C \in \mathscr{R}(A)$ and $D \in \mathscr{R}(B)$, $C \otimes D$ is a well-defined bounded operator on $\mathscr{H}_1 \otimes \mathscr{H}_2$ and $\|C \otimes D\| = \|C\| \, \|D\|$ (see the second proposition in Section VIII.10). We denote by $\mathscr{A}$ the norm closure in $\mathscr{L}(\mathscr{H}_1 \otimes \mathscr{H}_2)$ of the finite linear combinations of such operators $C \otimes D$. $\mathscr{A}$ is a commutative Banach algebra and the maps $A \mapsto A \otimes I$, $B \mapsto I \otimes B$ are isometric isomorphisms imbedding $\mathscr{R}(A)$ and $\mathscr{R}(B)$ into $\mathscr{A}$. If $\lambda \in \sigma(A \otimes B)$, then a fortiori λ is in the spectrum of $A \otimes B$ with respect to the algebra $\mathscr{A}$, so by the Gel'fand theory, there is a multiplicative linear functional ℓ on $\mathscr{A}$ so that $\lambda = \ell(A \otimes B) = \ell(A \otimes I)\ell(I \otimes B)$. Since the restrictions of ℓ to $\mathscr{R}(A) \otimes I$ and $I \otimes \mathscr{R}(B)$ are multiplicative, $\ell(A \otimes I) \in \sigma(A)$ and $\ell(I \otimes B) \in \sigma(B)$. This shows that

$$\sigma(A \otimes B) \subset \sigma(A)\sigma(B) \equiv \{\lambda_1 \lambda_2 \,|\, \lambda_1 \in \sigma(A), \lambda_2 \in \sigma(B)\} \tag{64}$$

In order to prove the reverse inclusion we shall have to work a little harder. First, we introduce a new subset of the spectrum.

Definition Let A be a closed linear operator on a Hilbert space $\mathscr{H}$. Let S denote the set of $\lambda \in \mathbb{C}$ so that for some $c_\lambda > 0$, $\|(A - \lambda)\varphi\| \geq c_\lambda \|\varphi\|$ for all $\varphi \in D(A)$. We define the **approximate point spectrum** by $\sigma_{\text{ap}}(A) \equiv \mathbb{C} \backslash S$. We also define $\sigma_r(A) \equiv \sigma(A) \backslash \sigma_{\text{ap}}(A)$.

$\sigma_{\text{ap}}(A)$ is called the approximate point spectrum because if $\lambda \in \sigma_{\text{ap}}(A)$, there is a sequence $\varphi_n \in D(A)$ with $\|\varphi_n\| = 1$ so that $(A - \lambda)\varphi_n \to 0$. The reader can check that σ_r is a subset of the residual spectrum defined in Section VI.3.

The following lemma summarizes two important properties of $\sigma_r(A)$.

Lemma 1

(a) If $\lambda \in \sigma_r(A)$, then $\bar{\lambda} \in \sigma_{\text{ap}}(A^*)$.
(b) $\sigma_r(A)$ is open.

Proof (a) is easy. For let $\lambda \in \sigma_r(A)$. Since $A - \lambda$ is not invertible but $\|(A - \lambda)\varphi\| \geq c_\lambda \|\varphi\|$ for some $c_\lambda > 0$, $\text{Ran}(\lambda - A)$ is not dense. Thus $\bar{\lambda}$ is in the point spectrum of A^*.

To prove (b), suppose that $\lambda \in \sigma_r(A)$. Then since $\|(A-\lambda)\varphi\| \geq c_\lambda \|\varphi\|$, $\mathrm{Ran}(A-\lambda)$ is a closed subspace of $\mathscr{H}$, but since $\lambda \in \sigma_r(A)$, $\mathrm{Ran}(A-\lambda) \neq \mathscr{H}$. Further, if $|z| \leq c_\lambda/2$, then $\|(A-(\lambda+z))\varphi\| \geq \frac{1}{2}c_\lambda\|\varphi\|$ so to prove that $\lambda + z \in \sigma_r(A)$ for z small enough we need only show that $\mathrm{Ran}(A-(\lambda+z)) \neq \mathscr{H}$. Suppose $\mathrm{Ran}(A-(\lambda+z)) = \mathscr{H}$ and let $\psi \in [\mathrm{Ran}(A-\lambda)]^\perp$ with $\|\psi\| = 1$. Then there is a $\varphi_z \in \mathscr{H}$ so that $(A-(\lambda+z))\varphi_z = \psi$ and $\|(A-(\lambda+z))\varphi_z\| \geq \frac{1}{2}c_\lambda\|\varphi_z\|$ if $|z| \leq c_\lambda/2$. Thus $\|\varphi_z\| \leq 2/c_\lambda$. In addition,

$$1 = \|\psi\|^2 = ((A-(\lambda+z))\varphi_z, \psi) = -z(\varphi_z, \psi) \leq |z|\|\varphi_z\| \leq |z|\frac{2}{c_\lambda}$$

For small z this is a contraction, so $\mathrm{Ran}(A-(\lambda+z)) \neq \mathscr{H}$ if z is small enough. ∎

Actually, as we have already noted in the proof of Theorem X.1, this proof of (b) shows that the codimension of $\mathrm{Ran}(A-\lambda)$ is constant on each component of $\sigma_r(A)$.

Lemma 2 Let A and B be bounded operators. Let $\langle \lambda_1, \lambda_2 \rangle$ be an interior point of $\sigma(A) \times \sigma(B)$ with $\lambda_1 \neq 0$. Then there is a point $\langle \lambda_1', \lambda_2' \rangle$ on the topological boundary of $\sigma(A) \times \sigma(B)$ so that $\lambda_1\lambda_2 = \lambda_1'\lambda_2'$.

Proof Let $s_1 = \sup\{t \in \mathbb{R} \mid t\lambda_1 \in \sigma(A)\}$, $s_2 = \sup\{t \in \mathbb{R} \mid \lambda_2/t \in \sigma(B)\}$, and $s = \min\{s_1, s_2\}$. Since A is bounded, $s_1 < \infty$ so $s < \infty$. Since either $s\lambda_1$ is on $\partial\sigma(A)$, the topological boundary of $\sigma(A)$, or λ_2/s is on $\partial\sigma(B)$, $\langle s\lambda_1, \lambda_2/s \rangle$ is on the topological boundary of $\sigma(A) \times \sigma(B)$. ∎

Theorem XIII.34 Let A and B be bounded operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively. Then $\sigma(A \otimes B) = \sigma(A)\sigma(B)$.

Proof We have already shown (64) so we need only show that $\sigma(A)\sigma(B) \subset \sigma(A \otimes B)$. Let $\lambda_1 \in \sigma(A)$ and $\lambda_2 \in \sigma(B)$. If $\lambda_1 = 0$, then it is easy to see that $0 \in \sigma(A \otimes B)$ so assume $\lambda_1 \neq 0 \neq \lambda_2$. By Lemma 2, we may assume that $\langle \lambda_1, \lambda_2 \rangle$ is on the topological boundary of $\sigma(A) \times \sigma(B)$. Without loss we assume $\lambda_1 \in \partial\sigma(A)$. Since $\sigma(A)$ is closed, $\lambda_1 \in \sigma(A)$. On the other hand, $\sigma_r(A)$ is open so $\lambda_1 \in \sigma_{ap}(A)$ and similarly, $\bar{\lambda}_1 \in \sigma_{ap}(A^*)$. There are now two cases to handle. Suppose $\lambda_2 \in \sigma_{ap}(B)$. Then there exist sequences $\varphi_n \in \mathscr{H}_1$, with $\|\varphi_n\| = 1$, $(A-\lambda_1)\varphi_n \to 0$, and $\psi_n \in \mathscr{H}_2$, with $\|\psi_n\| = 1$, $(B-\lambda_2)\psi_n \to 0$. Let $\eta_n = \varphi_n \otimes \psi_n$. Then

$$(A \otimes B - \lambda_1\lambda_2 I)\eta_n = (A-\lambda_1)\varphi_n \otimes B\psi_n + \lambda_1\varphi_n \otimes (B-\lambda_2)\psi_n$$

$$\to 0 \qquad \text{as} \quad n \to \infty$$

Thus, $\lambda_1 \lambda_2 \in \sigma_{ap}(A \otimes B)$. On the other hand, suppose that $\lambda_2 \in \sigma_r(B)$. Then $\bar{\lambda}_2 \in \sigma_{ap}(B^*)$ and $\bar{\lambda}_1 \in \sigma_{ap}(A^*)$. The same argument as above now shows that $\bar{\lambda}_1 \bar{\lambda}_2 \in \sigma_{ap}((A \otimes B)^*) \subset \sigma(A^* \otimes B^*)$. Thus $\lambda_1 \lambda_2 \in \sigma(A \otimes B)$ by Theorem VI.7. ∎

We shall use Theorem XIII.34 to prove that $\sigma(A \otimes I + I \otimes B) = \sigma(A) + \sigma(B)$ by first deriving spectral mapping formulas that relate the spectrum of the generator of a bounded holomorphic semigroup to the spectrum of its resolvent and the semigroup itself. Let C generate a bounded holomorphic semigroup on a Banach space X and define $\mathscr{C} \equiv \{e^{-tC} \mid t \geq 0\}''$ where $\{\cdot\}'$ denotes the commutant of a family of operators and $\{\cdot\}''$ the double commutant. Explicitly,

$$\mathscr{A}' = \{B \mid AB = BA \text{ for all } A \in \mathscr{A}\}$$

$$\mathscr{A}'' = \{\mathscr{A}'\}'$$

Lemma 3 If C is the generator of a bounded holomorphic semigroup, then

$$\mathscr{C} \equiv \{e^{-tC} \mid t \geq 0\}'' = \{R_\lambda(C) \mid \lambda \in \rho(C)\}''$$

Moreover, $\mathscr{C}$ is an abelian Banach algebra.

Proof It is sufficient to prove that

$$\{e^{-tC} \mid t \geq 0\}' = \{R_\lambda(C) \mid \lambda \in \rho(C)\}'$$

This follows easily from (X.98)

$$(\lambda + C)^{-1}\varphi = \int_0^\infty e^{-\lambda t} e^{-tC} \varphi \, dt$$

and (X.102)

$$e^{-zC} = -\frac{1}{2\pi i} \int_\Gamma e^{-\lambda z}(\lambda - C)^{-1} \, d\lambda$$

where Γ is a suitable path.

The last statement in the lemma is a general fact about operator algebras. Since $\{e^{-tC} \mid t \geq 0\}$ is abelian, $\{e^{-tC} \mid t \geq 0\} \subset \{e^{-tC} \mid t \geq 0\}'$. Thus, $\{e^{-tC} \mid t \geq 0\}'' \subset \{e^{-tC} \mid t \geq 0\}'$. Therefore if A and B are in $\{e^{-tC} \mid t \geq 0\}''$, A is also in $\{e^{-tC} \mid t \geq 0\}'$ so A and B commute. ∎

Since $\mathscr{C}$ is a commutant, it has the following very important property: The Gel'fand spectrum with respect to the algebra of each $D \in \mathscr{C}$ is the same as its spectrum as an operator on X. This is because if D commutes with

$\{e^{-tC} \mid t > 0\}'$, then all the resolvents of D also commute with $\{e^{-tC} \mid t > 0\}'$, so they are all in $\mathscr{C}$. Therefore, for an element D in $\mathscr{C}$ we shall just write $\sigma(D)$ for its spectrum with respect to $\mathscr{C}$.

The following is essentially a restatement of Lemma 2 from Section 4.

Lemma 4 Let C be a closed operator with nonempty resolvent set on a Banach space X. Suppose that $\lambda \in \rho(C)$ and regard $h: z \mapsto (\lambda - z)^{-1}$ as a map of the extended complex plane onto itself. Then:

(a) If C is bounded, h is a homeomorphism of $\sigma(C)$ onto $\sigma((\lambda - C)^{-1})$.
(b) If C is unbounded, h is a homeomorphism of $\sigma(C) \cup \{\infty\}$ onto $\sigma((\lambda - C)^{-1})$.

We can now prove a spectral mapping theorem for the semigroup generated by C.

Lemma 5 Let C be the generator of a bounded holomorphic semigroup on a Banach space X. Then:

(a) $\sigma(e^{-tC}) = e^{-t\sigma(C)} \equiv \{e^{-tz} \mid z \in \sigma(C)\}$ if C is bounded.
(b) $\sigma(e^{-tC}) = e^{-t\sigma(C)} \cup \{0\}$ if C is unbounded.

Proof If $\ell \in \sigma(\mathscr{C})$, the set of multiplicative linear functionals on $\mathscr{C}$, then the first resolvent equation shows that either $\ell((\lambda - C)^{-1}) = 0$ for all $\lambda \in \rho(C)$ or for no $\lambda \in \rho(C)$. Let $\mathscr{M}_\infty = \{\ell \in \sigma(\mathscr{C}) \mid \ell((\lambda - C)^{-1}) = 0\}$ and $\mathscr{M}_0 = \sigma(\mathscr{C}) \backslash \mathscr{M}_\infty$. For $\ell \in \mathscr{M}_0$, we define

$$\hat{C}(\ell) \equiv \lambda - [\ell((\lambda - C)^{-1})]^{-1}$$

It follows from the first resolvent equation that this definition is independent of which $\lambda \in \rho(C)$ is chosen. Since $\ell((\lambda - C)^{-1}) = 0$ if $\ell \in \mathscr{M}_\infty$ and

$$\ell((\lambda - C)^{-1}) = (\lambda - \hat{C}(\ell))^{-1}, \qquad \ell \in \mathscr{M}_0$$

it follows that $\sigma((\lambda - C)^{-1}) = \{(\lambda - \hat{C}(\ell))^{-1} \mid \ell \in \mathscr{M}_0\} \cup \{0\}$ in the case where C is unbounded. Thus by Lemma 4, $\sigma(C) = \operatorname{Ran} \hat{C} \restriction \mathscr{M}_0$. The same holds if C is bounded. Now, suppose that $\ell \in \mathscr{M}_0$, then by (X.102)

$$\begin{aligned} \ell(e^{-tC}) &= \frac{-1}{2\pi i} \int_\Gamma e^{-\lambda t} \ell((\lambda - C)^{-1})\, d\lambda \\ &= e^{-\lambda \hat{C}(\ell)} \end{aligned}$$

by Cauchy's theorem. If $\ell \in \mathscr{M}_\infty$, the same formula shows that $\ell(e^{-tC}) = 0$ for all $t > 0$. Since $\sigma(e^{-tC}) = \{\ell(e^{-tC}) \mid \ell \in \sigma(\mathscr{C})\}$, we conclude that $\sigma(e^{-tC}) = e^{-t\sigma(C)} \cup \{0\}$ if C is unbounded and $\sigma(e^{-tC}) = e^{-t\sigma(C)}$ if C is bounded. ∎

The following theorem and its proof extend to the Banach space case. We state and prove it only in the Hilbert space case since we have not discussed the tensor product of Banach spaces and the Hilbert space case is all we need in Section 10.

Theorem XIII.35 Let A and B be the generators of bounded holomorphic semigroups on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. Let C be the closure of the operator $A \otimes I + I \otimes B$ defined on $D(A) \otimes D(B)$. Then C generates a bounded holomorphic semigroup and

$$\sigma(C) = \sigma(A) + \sigma(B)$$

Proof Suppose that e^{-zA} and e^{-zB} are bounded holomorphic semigroups of angle θ_1 and θ_2, respectively. Then $W(z) = e^{-zA} \otimes e^{-zB}$ is a bounded holomorphic semigroup of angle $\theta = \min\{\theta_1, \theta_2\}$. Let G be the generator of $W(z)$. $W(t)$ is strongly differentiable on $D(A) \otimes D(B)$ and $G \upharpoonright D(A) \otimes D(B) = A \otimes I + I \otimes B$. Since $W(z)$: $D(A) \otimes D(B) \to D(A) \otimes D(B)$, Theorem X.49 implies that $D(A) \otimes D(B)$ is a core for G. Thus $G = C$.

By Theorem XIII.34, $\sigma(e^{-tC}) = \sigma(e^{-tA})\sigma(e^{-tB})$. Therefore, by Lemma 5,

$$e^{-t\sigma(C)} = \tilde{\sigma}(e^{-tC}) = \tilde{\sigma}(e^{-tA})\tilde{\sigma}(e^{-tB}) = e^{-t(\sigma(A)+\sigma(B))}$$

where $\tilde{\sigma}(\cdot)$ denotes $\sigma(\cdot)\backslash\{0\}$. Thus, if $\mu \in \sigma(A)$ and $\lambda \in \sigma(B)$, then for all t there is a $\gamma_t \in \sigma(C)$ so that $e^{-t\gamma_t} = e^{-t(\mu+\lambda)}$, i.e., $\gamma_t = \mu + \lambda + t^{-1}2\pi i n_t$ where n_t is an integer. Since $\gamma_t \in \overline{S}_{\frac{1}{2}\pi-\theta} = \{z \mid |\arg z| \leq \frac{1}{2}\pi - \theta\}$, n_t must be zero if t is small enough. Thus, $\gamma = \mu + \lambda \in \sigma(C)$. Conversely, suppose $\gamma \in \sigma(C)$. Then, for each t, there is a $\mu_t \in \sigma(A) \subset \overline{S}_{\frac{1}{2}\pi-\theta}$ and a $\lambda_t \in \sigma(B) \subset \overline{S}_{\frac{1}{2}\pi-\theta}$ so that $\gamma = \mu_t + \lambda_t + t^{-1}2\pi i n_t'$ where n_t' is an integer. Since $\gamma, \mu_t, \lambda_t \in \overline{S}_{\frac{1}{2}\pi-\theta}$ we again see that if t is small $\gamma = \mu_t + \lambda_t$. Thus $\sigma(C) = \sigma(A) + \sigma(B)$. ∎

Corollary 1 If A and B are bounded operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, then

$$\sigma(A \otimes I + I \otimes B) = \sigma(A) + \sigma(B)$$

Proof $A + 2\|A\|$ and $B + 2\|B\|$ generate bounded holomorphic semigroups so by the above theorem,

$$\begin{aligned}
&\sigma(A \otimes I + I \otimes B) + 2\|A\| + 2\|B\| \\
&\quad = \sigma((A + 2\|A\|) \otimes I + I \otimes (B + 2\|B\|)) \\
&\quad = \sigma(A + 2\|A\|) + \sigma(B + 2\|B\|) \\
&\quad = \sigma(A) + \sigma(B) + 2\|A\| + 2\|B\| \quad ∎
\end{aligned}$$

Corollary 2 (Ichinose's lemma) Let $\bar{S}_{\omega,\varphi,\theta}$ denote the sector $\{z \mid \varphi - \theta \leq \arg(z-\omega) \leq \varphi + \theta; \theta < \pi/2\}$. Let A and B be strictly m-sectorial operators on Hilbert space $\mathscr{H}_1$ and $\mathscr{H}_2$ with sectors $\bar{S}_{\omega_1,\varphi,\theta_1}$ and $\bar{S}_{\omega_2,\varphi,\theta_2}$ (same φ!). Let C denote the closure of $A \otimes I + I \otimes B$ on $D(A) \otimes D(B)$. Then C is a strictly m-sectorial operator with sector $S_{\omega_1+\omega_2,\varphi,\min\{\theta_1,\theta_2\}}$ and $\sigma(C) = \sigma(A) + \sigma(B)$.

Proof The proof follows immediately by translating and rotating A and B so that they become strictly m-accretive and then applying Corollary 1 of Theorem X.52 and the above theorem. ∎

XIII.10 The absence of singular continuous spectrum IV: Dilation analytic potentials

Thus far, we have proven the absence of singular continuous spectrum for three types of Schrödinger operators: a wide range of two-body operators, n-body systems with repulsive potentials, and n-body systems with weak potentials. All these systems have the property of possessing only one scattering channel; equivalently, their subsystems have no bound states. In this section we discuss a method for proving the absence of singular continuous spectrum in multichannel n-body systems with $n \geq 3$. The class of pair interactions that we can treat is very restrictive but it does include Coulomb and generalized Yukawa potentials.

Definition The group of unitary operators $u(\theta)$ on $L^2(\mathbb{R}^3)$ given by

$$(u(\theta)\psi)(r) = e^{3\theta/2}\psi(e^{\theta}r)$$

is called the **group of dilation operators on** $\mathbb{R}^3$.

The factor $e^{3\theta/2}$ is included to make u unitary. Throughout this section we use $u(\theta)$ to stand for this family of operators.

The idea behind using dilations for spectral analysis is the following. The kinetic energy $H_0 = -\Delta$ transforms very simply under dilations; in fact,

$$u(\theta)H_0\,u(\theta)^{-1} = e^{-2\theta}H_0 \equiv H_0(\theta)$$

This last expression implies that $u(\theta)H_0\,u(\theta)^{-1}$, defined a priori when θ is real, has an analytic continuation to complex θ. We shall restrict our potentials so that the same is true when $H = -\Delta + V$ replaces H_0. We shall see below that $H(\theta)$ has a discrete spectrum that is "locally" independent of θ.

However as is clear from the case of H_0 where $\sigma(H_0(\theta)) = \{z \,|\, \arg z = -2 \operatorname{Im} \theta\}$, the continuous spectrum changes considerably as θ varies. This allows one to separate the continuous spectrum from the real axis:

Definition Let $\alpha > 0$. A quadratic form V on $L^2(\mathbb{R}^3)$ is said to be in class $\mathscr{F}_\alpha$ if and only if:

(1) V is a symmetric form with $Q(V) \supset Q(H_0)$ where $H_0 = -\Delta$.
(2) $(H_0 + I)^{-1/2} V (H_0 + I)^{-1/2}$ is compact.
(3) The family of operators

$$F(\theta) = (H_0 + I)^{-1/2}(u(\theta) V u(\theta)^{-1})(H_0 + I)^{-1/2}$$

defined for $\theta \in \mathbb{R}$ has an extention to an analytic bounded operator-valued function into the strip B_α where

$$B_\alpha \equiv \{\theta \,|\, |\operatorname{Im} \theta| < \alpha\}$$

The set $\bigcup_{\alpha > 0} \mathscr{F}_\alpha$ is called the family of **dilation analytic potentials.**

If the function $F(\theta)$ in (3) has an extension to $\{\theta \,|\, |\operatorname{Im} \theta| \leq \alpha\}$ analytic in the interior and norm continuous up to the boundary, we say that V is in class $\overline{\mathscr{F}}_\alpha$.

In the above definition $u(\theta) V u(\theta)^{-1} \equiv V(\theta)$ denotes the quadratic form $V(\theta)(\psi, \varphi) = V(u(-\theta)\psi, u(-\theta)\varphi)$. The definition of dilation analytic potentials can be conveniently rephrased in terms of the scale of spaces $\mathscr{H}_{+1} \subset \mathscr{H} \subset \mathscr{H}_{-1}$ defined by the quadratic form of H_0 (see Section VIII.6). For (1) and (2) say that V defines a compact operator from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$ that is self-dual. To state (3), we first note that

$$(H_0 + 1)^{1/2} u(\theta)(H_0 + 1)^{-1/2} = (H_0 + 1)^{1/2}(e^{-2\theta} H_0 + 1)^{-1/2} u(\theta)$$

so that $u(\theta)$ defines a bounded map from $\mathscr{H}_{+1}$ to $\mathscr{H}_{+1}$ and, since $u(-\theta)^* = u(\theta)$, from $\mathscr{H}_{-1}$ to $\mathscr{H}_{-1}$. Thus, since V is bounded from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$, for any real θ, $u(\theta) V u(\theta)^{-1}$ is defined as a compact operator from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$. Statement (3) then says that this function has an $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$-valued analytic continuation.

When V is dilation analytic and $\operatorname{Im} \theta < \alpha$, we shall let $V(\theta)$ denote the quadratic form associated with the operator in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ obtained by the above continuation. Since the above argument shows that $V(\theta)$ is a compact operator from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$ when θ is real and since the analytic continuation of an operator-valued function with compact values on the real

axis is compact (Lemma 5 in Section 5), we conclude that $V(\theta)$ is a relatively form compact perturbation of H_0 for all θ and in particular, it is a form-bounded perturbation with relative bound zero (see Problem 38). As a result, we have the following:

Proposition 1 Let $V \in \mathscr{F}_\alpha$ and let $H_0 = -\Delta$. Let $H_0(\theta) = e^{-2\theta}H_0$ for $\theta \in B_\alpha$. Define the quadratic form $H(\theta) = H_0(\theta) + V(\theta)$ on $Q(H_0)$ as the sum of the forms $H_0(\theta)$ and $V(\theta)$. Then:

(a) For any $\theta \in B_\alpha$, $H(\theta)$ is a strictly m-sectorial form; explicitly, for any ε, there is a z_0 so that

$$S_{z_0,\,\mathrm{Im}\,\theta,\,\varepsilon} = \{\omega \,|\, 2\,\mathrm{Im}\,\theta - \varepsilon < \arg(\omega - z_0) < 2\,\mathrm{Im}\,\theta + \varepsilon\}$$

is a sector for $H(\theta)$.

(b) $H(\theta)$ is an analytic family of type (B) in the region B_α.

(c) For any real φ, $u(\varphi)H(\theta)u(\varphi)^{-1} = H(\theta + \varphi)$.

Proof Let $A(\theta) \equiv e^{2\theta}H(\theta) = H_0 + e^{2\theta}V(\theta)$. Since H_0 is self-adjoint and $e^{2\theta}V(\theta)$ is a form-bounded perturbation of H_0 with relative bound 0, for any δ, we can find b so that

$$|(\varphi, e^{2\theta}V(\theta)\varphi)| < \delta(\varphi, (H_0 + b)\varphi)$$

Letting $\varepsilon = \sin^{-1}\delta$, we have $\arg[(\varphi, (H_0 + e^{2\theta}V(\theta) + b)\varphi)] < \varepsilon$. This proves (a). $A(\theta)$ is clearly analytic of type (B) so the same is true of $H(\theta)$. To prove (c), fix $\varphi \in \mathbb{R}$ and note that $u(\varphi)H(\theta)u(\varphi)^{-1}$ and $H(\theta + \varphi)$ are both analytic in B_α and they are clearly equal if $\theta \in \mathbb{R}$. ∎

Before turning to some examples, we note that there is an operator version of dilation analytic potentials, but that the related class $\mathscr{C}_\alpha$ is contained in $\mathscr{F}_\alpha$ (see Problem 73).

Example 1 Let V be a central potential given by a real-valued function $V(r)$. Then, for real θ, $V(\theta)$ is multiplication by the function $V(e^\theta r)$. It is now easy to see (Problem 74) that if $V(r)$ has an analytic continuation $V(z)$ to a sector $\{z \,|\, |\arg z| < \alpha\}$ with

$$\lim_{\substack{|z|\to\infty \\ |\arg z|<\beta}} V(z) = 0$$

and

$$\sup_{0<|\varphi|<\beta} \int_{|r|,\,|r'|\le 1} |V(e^{i\varphi}r)|\,|V(e^{i\varphi}r')|\,|r - r'|^{-2}\,d^3r\,d^3r' < \infty$$

for each $\beta < \alpha$, then V is dilation analytic. In fact, for each $\theta \in B_\alpha$, $V(\theta)$ is multiplication by $V(e^\theta r)$ which is in $R + (L^\infty)_\varepsilon$. In particular, the Coulomb potential $V(r) = r^{-1}$ is in $\mathscr{F}_\infty$ and the Yukawa potential $V(r) = e^{-\mu r}/r$, $\mu > 0$, is in $\overline{\mathscr{F}}_{\pi/2}$.

Example 2 Dilation analytic potentials need not be "local," i.e., they do not have to be multiplication operators. For example, let $\psi \in L^2$ be an analytic vector for the infinitesimal generator of $u(\theta)$. Thus $\{u(\theta)\psi\}_{\theta \in \mathbb{R}}$ has an analytic continuation to a strip $\{\theta \,|\, |\operatorname{Im} \theta| < \alpha\}$ (Problem 75). Let V be the rank-one operator $(\psi, \cdot)\psi$. Then V is dilation analytic; in fact $V(\theta) = (\psi(\bar{\theta}), \cdot)\psi(\theta)$.

Our ultimate goal in this section is to analyze the spectrum of the Hamiltonian H on $L^2(\mathbb{R}^{3N-3})$ obtained by removing the center of mass from $\tilde{H} = -\sum_{i=1}^N (2\mu_i)^{-1}\Delta_i + \sum_{i<j} V_{ij}(r_i - r_j)$ where each V_{ij} is an operator on $L^2(\mathbb{R}^3)$ that is dilation analytic. We begin by considering the two-body case and then use the method of the two-body case in the general situation supplementing it with the Weinberg–Van Winter equations and Ichinose's lemma.

Theorem XIII.36 Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and let $V \in \mathscr{F}_\alpha$ for some $\alpha > 0$. Suppose that $\theta \in B_\alpha$ and let $H(\theta) = e^{-2\theta}H_0 + V(\theta)$. Then:

(a) $\sigma(H(\theta))$ is only dependent on $\operatorname{Im} \theta$.
(b) $\sigma(H(\theta))$ consists of $\{e^{-2\theta}\lambda \,|\, \lambda \in [0, \infty)\} \cup \sigma_{\mathrm{d}}(\theta)$ where σ_{d} is a set whose only possible limit point is zero. Each $\mu \in \sigma_{\mathrm{d}}(\theta)$ is an eigenvalue of finite multiplicity.
(c) $\sigma_{\mathrm{d}}(\bar{\theta}) = \overline{\sigma_{\mathrm{d}}(\theta)}$.
(d) If $0 < \operatorname{Im} \theta < \frac{1}{2}\pi$, then $\sigma_{\mathrm{d}}(\theta) \subset \mathbb{R} \cup \{\mu \,|\, -2 \operatorname{Im} \theta < \arg \mu < 0\}$ and $\mathbb{R} \cap \sigma_{\mathrm{d}}(\theta) = \sigma_{\mathrm{pp}}(H(0)) \backslash \{0\}$. Moreover, if $0 < \operatorname{Im} \varphi < \operatorname{Im} \theta < \frac{1}{2}\pi$, then $\sigma_{\mathrm{d}}(\varphi) \subset \sigma_{\mathrm{d}}(\theta)$.
(e) $\sigma_{\mathrm{sing}}(H(0)) = \varnothing$.

Proof (a) and (c) follow from Proposition 1 which says that $H(\theta)$ and $H(\theta + \varphi)$ are unitarily equivalent if $\varphi \in \mathbb{R}$ and $H(\theta)^* = H(\bar{\theta})$. Corollary 2 to Theorem XIII.14 implies that $\sigma_{\mathrm{ess}}(e^{2\theta}H(\theta)) = \sigma_{\mathrm{ess}}(H_0) = [0, \infty)$. This proves (b) except that a priori $\sigma_{\mathrm{d}}(\theta)$ could have limit points anywhere in $e^{-2\theta}\mathbb{R}_+$. This leaves (d) and (e). Fix θ_0 and suppose that $E \in \sigma_{\mathrm{d}}(\theta_0)$. Since $H(\theta)$ is an analytic family of type (B), Theorem XII.13 implies that for θ near θ_0, $H(\theta)$ has eigenvalues near E and that these nearby eigenvalues are given by all the branches of one or more functions $f_1(\theta), \ldots, f_n(\theta)$ analytic near θ_0 with at

worst algebraic branch points near θ_0. On the other hand, if φ is real, $H(\theta_0)$ and $H(\theta_0 + \varphi)$ are unitarily equivalent, so the only eigenvalue of $H(\theta_0 + \varphi)$ near E is E. We conclude that $f_i(\theta) = E$ if θ is near θ_0 and $\theta - \theta_0$ is real. But analyticity then implies that $f_i(\theta) = E$ for the entire region where f is defined! Thus we have proven that $\sigma_d(\theta)$ is locally constant in the sense that if $\lambda \in \sigma_d(\theta_0)$, then it is in $\sigma_d(\theta)$ for all θ near θ_0. On the other hand, if $\theta_n \to \theta$ and $\lambda \in \sigma_d(\theta_n)$ for each n, then $\lambda \in \sigma(H(\theta))$ since $H(\theta_n) \to H(\theta)$ in norm resolvent sense. Therefore a simple connectedness argument (Problem 76) proves the following statement: If $\gamma(t)$ $(0 \leq t \leq 1)$ is a curve in B_α and $\lambda \in \sigma_d(\gamma(0))$, then either $\lambda \in \sigma_d(\gamma(1))$ or $\lambda \in \sigma_{ess}(H(\gamma(t)))$ for some $t \in (0, 1]$. In particular, if $\lambda \notin \{\mu \mid -2 \operatorname{Im} \theta \leq \arg \mu \leq 0\}$ and if $0 < \operatorname{Im} \theta < \frac{1}{2}\pi$, then $\lambda \in \sigma_d(\theta)$ if and only if $\lambda \in \sigma_d(0)$ for we can take the curve $\gamma(t) = t\theta$. Thus

$$\sigma_d(\theta) \cap \{\mu \mid 0 < \arg \mu < 2\pi - 2 \operatorname{Im} \theta\} = \sigma_{pp}(H) \cap (-\infty, 0)$$

Similarly, if $0 < \operatorname{Im} \varphi < \operatorname{Im} \theta$, then $\sigma_d(\varphi) \subset \sigma_d(\theta)$. This shows that $\sigma_d(\theta)$ cannot have any limit points other than zero. To complete the proof of (d), we need only show that $\sigma_d(\theta) \cap (0, \infty) = \sigma_{pp}(H) \cap (0, \infty)$. This requires an additional idea which is also needed for the proof of (e). Let

$$N_\alpha = \{\psi \in L^2(\mathbb{R}^3) \mid u(\theta)\psi \text{ has an analytic continuation from } \mathbb{R} \text{ to } B_\alpha\}$$

N_α is precisely the set of analytic vectors ψ for the infinitesimal generator D of $u(\theta)$ for which $\sum_{n=0}^{\infty} t^n \|D^n\psi\|/n!$ has radius of convergence at least α. Let $\psi \in N_\alpha$ and let $\psi(\theta)$ denote the continuation of $u(\theta)\psi$. Consider the function $f(z, \theta) = (\psi(\bar{\theta}), (H(\theta) - z)^{-1}\psi(\theta))$. For each fixed $\theta \in B_\alpha$, $f(z, \theta)$ is analytic in z for $z \in \mathbb{C}\backslash\sigma(H(\theta))$ and meromorphic in $\mathbb{C}\backslash\sigma_{ess}(\theta)$. On the other hand, let us fix z with $\operatorname{Im} z > 0$. Then $f(z, \theta)$ is analytic in θ in the region

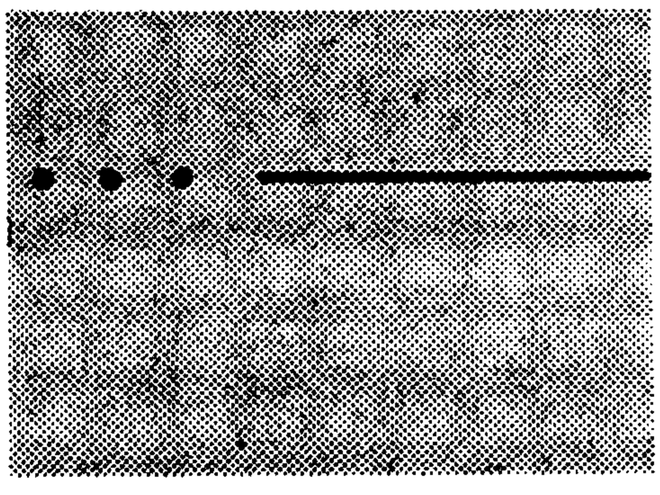
$$R_z = \{\theta \mid -\min\{\alpha, \tfrac{1}{2} \arg z\} < \operatorname{Im} \theta < \min\{\alpha, \tfrac{1}{2}\pi\}\}.$$

Since for $\varphi \in \mathbb{R}$,

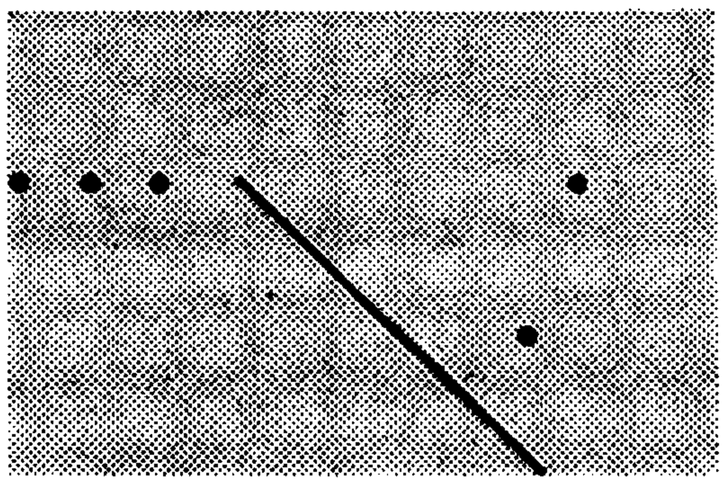
$$\begin{aligned} f(z, \varphi) &= (u(\varphi)\psi, (H(\varphi) - z))^{-1}u(\varphi)\psi) = (u(\varphi)\psi, u(\varphi)(H(0) - z)^{-1}\psi) \\ &= f(z, 0) \end{aligned}$$

we conclude by analyticity that $f(z, \cdot)$ is constant in R_z. In particular, if $0 < \operatorname{Im} \theta_0 < \min\{\alpha, \frac{1}{2}\pi\}$, then $f(z, \theta_0)$ provides an analytic continuation of $f(z, 0)$ from $\mathbb{C}\backslash\sigma(H(0))$ to $\mathbb{C}\backslash\sigma(H(\theta_0))$ (see Figure XIII.5). In particular, if $\psi \in N_\alpha$, then $(\psi, (H - z)^{-1}\psi)$ has continuous boundary values as $z \to \mu + i0$ if $\mu \in \mathbb{R}\backslash\sigma_d(\theta_0)$. Since N_α is dense, and $\sigma_d(\theta_0) \cap \mathbb{R}$ is discrete, we conclude that $\sigma_{sing}(H(0)) = \varnothing$ by appealing to Theorem XIII.20.

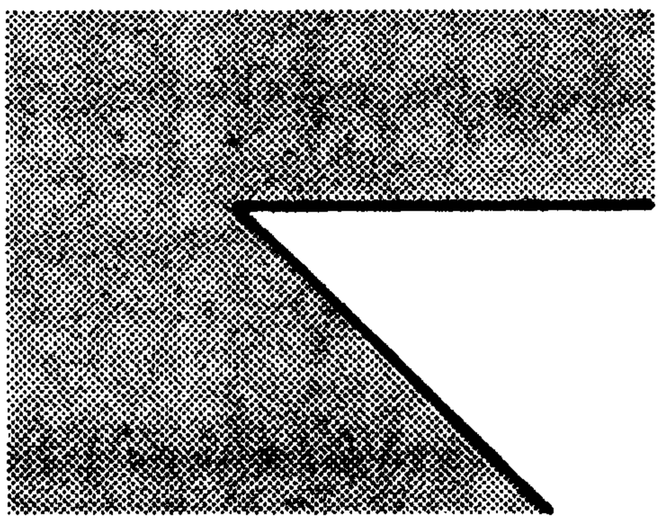
Finally, we return to the proof that $\sigma_d(\theta) \cap (0, \infty) = \sigma_{pp}(H(0)) \cap (0, \infty)$ if $0 < \operatorname{Im} \theta < \min\{\alpha, \frac{1}{2}\pi\}$. Since $H(0)$ is self-adjoint, the functional calculus immediately implies that $\text{s-lim}_{\varepsilon \downarrow 0}\ i\varepsilon(H - x - i\varepsilon)^{-1} = P_{\{x\}}$ for any $x \in \mathbb{R}$.



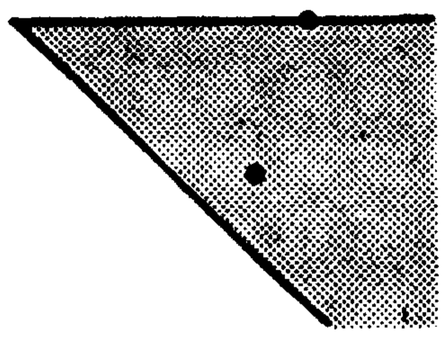
(a) Domain of $f(z, 0)$



(b) Domain of $f(z, \theta)$



(c) Region of agreement



(d) Region gained by dilation analyticity

FIGURE XIII.5 Analytic continuation of matrix elements of the resolvent.

Suppose that $x \notin \sigma_d(\theta) \cap (0, \infty)$. Then, by the above argument, $(\psi, (H - z)^{-1}\psi)$ has an analytic continuation from $\{z \,|\, \text{Im } z > 0\}$ to a neighborhood of x if $\psi \in N_\alpha$. In particular, $\lim_{\varepsilon \downarrow 0} i\varepsilon(\psi, (H - x - i\varepsilon)^{-1}\psi) = 0$ so $P_{\{x\}}\psi = 0$. Since N_α is dense, $P_{\{x\}} = 0$, i.e., $x \notin \sigma_{pp}(H(0)) \cap (0, \infty)$. Conversely, let $x \in \sigma_d(\theta) \cap (0, \infty)$. Let η be an eigenvector for $H(\theta)$ with eigenvalue x. Then $(\varphi, (H(\theta) - z)^{-1}\eta)$ has a pole at $z = x$ for some φ. Since $N_{2\alpha}$ is dense, we can find φ_n, $\eta_n \in N_{2\alpha}$ so that $\varphi_n \to \varphi$, $\eta_n \to \eta$. For $z \notin \sigma(H(\theta))$, $(\varphi_n, (H(\theta) - z)^{-1}\eta_n)$ converges to $(\varphi, (H(\theta) - z)^{-1}\eta)$; so, by the argument principle (which relates the number of poles of a meromorphic function inside a contour to the integral of f'/f on the contour), we conclude that for all large n, $(\varphi_n, (H(\theta) - z)^{-1}\eta_n)$ has a pole at $z = x$. Let $\psi = \eta_n(-\theta)$, $\kappa = \varphi_n(-\theta)$. Then $(\psi, (H - z)^{-1}\kappa) = (\varphi_n, (H(\theta) - z)^{-1}\eta_n)$ if $\text{Im } z > 0$ so we conclude that $(\psi, (H - z)^{-1}\kappa)$ has a pole at $z = x$. Thus $(\psi, P_{\{x\}}\kappa) \neq 0$ and therefore $x \in \sigma_{pp}(H)$. ∎

In the above proof a critical role was played by the fact that we could explicitly find $\sigma_{ess}(H(\theta))$ on account of Weyl's theorem. In the N-body case, we have to replace Weyl's theorem with a theorem of the same type as the HVZ theorem. There is one important difference between what we need now to analyze $H(\theta)$ and the analysis of Section 5—namely the potentials $V_{ij}(\theta)$ are not self-adjoint. As preparation for an N-body analogue to Theorem XIII.36, we therefore prove:

Proposition 2 Let $\tilde{H} = \tilde{H}_0 + \sum_{1 \le i < j = N} \tilde{V}_{ij}$ where:

(i) $\tilde{H}_0 = \sum_{i=1}^{N} (2\mu_i)^{-1} \Delta_i$.

(ii) Under the decomposition induced by writing $\mathbb{R}^{3N} = \mathbb{R}^3 \times \mathbb{R}^{3N-3}$ with $\mathbb{R}^3$ corresponding to the coordinate $r_i - r_j$, $\tilde{V}_{ij} = V_{ij} \otimes I$.

(iii) Each V_{ij} is a relatively form compact perturbation of $-\Delta$ on $L^2(\mathbb{R}^3)$, but is not necessarily symmetric.

Let H be $\tilde{H}$ with its center of mass removed. For each cluster $C \subset \{1, \ldots, N\}$, define $H(C_i)$ according to the prescription in Section XI.5. For each cluster decomposition $D = \{C_1, \ldots, C_k\}$ call the family of numbers $\{E_1 + \cdots + E_k \,|\, E_i \in \sigma_{\text{disc}}(H(C_i))\}$ the set of **D-thresholds**, written Σ_D. Let Σ denote the union of the Σ_D over all D with at least two clusters. Then

$$\sigma_{\text{ess}}(H) \subset \bigcup_{\lambda \in \Sigma} (\lambda + [0, \infty))$$

Proof We shall only indicate the changes necessary in the argument in Section 5; the details are left to the reader (Problem 77). If $N = 2$, then $\Sigma = \{0\}$ and the conclusion of the theorem is part of Weyl's essential spectrum theorem. Thus we can suppose that the theorem holds for all M-body systems with $M \le N - 1$ and prove it for N-body systems. The first step is to prove that

$$\sigma(H_D) \subset \bigcup_{\lambda \in \Sigma} (\lambda + [0, \infty)) \tag{65}$$

for any D with at least two clusters. To see this, write $D = \{C_1, \ldots, C_k\}$ so that $H_D = \sum_{i=1}^{k} H(C_i) + T_D$. Now, each V_{ij} is a form-bounded perturbation of H_0 with relative bound zero so each $H(C_i)$ is a strictly m-sectorial operator with arbitrarily small opening angle. Moreover, under the natural decomposition $\mathscr{H} \equiv L^2(\mathbb{R}^{3N-3}) = \mathscr{H}_D \otimes \mathscr{H}_{C_1} \otimes \cdots \otimes \mathscr{H}_{C_k}$ each summand of $\sum_{i=1}^{k} H(C_i) + T_D$ acts on a different factor in the tensor product. As a consequence, Ichinose's lemma (Theorem XIII.35 and its corollary) is applicable and $\sigma(H_D) = \sum_{i=1}^{k} \sigma(H(C_i)) + \sigma(T_D)$. Using the fact that $\sigma(H(C_i)) = \sigma_{\text{disc}}(H(C_i)) \cup \sigma_{\text{ess}}(H(C_i))$ and the inductive hypothesis, it is easy to prove (65).

At this point one can mimic the proof of the HVZ theorem fairly closely. Since $\sum V_{ij}$ is a form-bounded perturbation of relative bound zero, the perturbation series for $G(E) = (H_0 + \sum V_{ij} - E)^{-1}$ converges in norm if E is very negative. Writing $R(E) = (H_0 - E)^{+1/2} G(E)(H_0 - E)^{1/2}$, we can resum $R(E) = D_R(E) + I_S(E)R(E)$ as in Section 5. Both $D_R(E)$ and $I_S(E)$ can be expressed in terms of resolvents for $(H_D - E)^{-1}$ where D has at least two clusters. By our analysis above, they both have analytic continuations to $\mathbb{C} \backslash S$ where $S = \bigcup_{\lambda \in \Sigma} (\lambda + [0, \infty))$. This step requires one to use the induction

hypothesis to conclude that S is closed. Finally, one shows that each connected diagram is compact, uses this to prove $I_S(E)$ is compact, and employs the analytic Fredholm theorem to complete the proof. ∎

At this point it is easy to prove the main result of this section. For ease of statement, we first define:

Definition Let $V_{ij} \in \mathscr{F}_\alpha$ for each pair $1 \leq i < j \leq N$ and let $\tilde{V}_{ij} = V_{ij} \otimes I$ on $L^2(\mathbb{R}^{3N})$ in terms of the decomposition $\mathbb{R}^{3N} = \mathbb{R}^3 \times \mathbb{R}^{3N-3}$ where the first coordinate is $r_i - r_j$. Let $\tilde{H}_0 = -\sum_{i=1}^{N} (2\mu_i)^{-1} \Delta_i$ and let $\tilde{H} = \tilde{H}_0 + \sum \tilde{V}_{ij}$ For $\theta \in B_\alpha$, let $\tilde{H}(\theta) = e^{-2\theta} \tilde{H}_0 + \sum \tilde{V}_{ij}(\theta)$. Let $H(\theta)$ and H denote $\tilde{H}(\theta)$, $\tilde{H}$ with their center of mass motion removed. For every cluster decomposition $D = \{C_1, \ldots, C_k\}$, let $\Sigma_D(\theta) \equiv \{E_1 + \cdots + E_k \,|\, E_i \in \sigma_{\text{disc}}(H_{C_i}(\theta))\}$ and let $\Sigma(\theta) = \bigcup_{\#(D) \geq 2} \Sigma_D(\theta)$. Finally we let $\Sigma_{\min} = \min\{\lambda \,|\, \lambda \in \Sigma(0)\}$.

Theorem XIII.37 Let H be an N-body Hamiltonian on $L^2(\mathbb{R}^{3N-3})$ with dilation analytic pair potentials of the type described in the last definition. Then:

(a) $\sigma(H(\theta))$ and $\Sigma(\theta)$ depend only on $\operatorname{Im} \theta$.

(b) $\sigma(H(\theta)) = \sigma_{\text{ess}}(\theta) \cup \sigma_{\text{d}}(\theta)$ where the essential spectrum $\sigma_{\text{ess}}(\theta) = \{\mu + e^{-2\theta}\lambda \,|\, \mu \in \Sigma(\theta), \lambda \in [0, \infty)\}$ and where $\sigma_{\text{d}}(\theta)$ is the discrete spectrum of $\sigma(H(\theta))$.

(c) $\sigma_{\text{d}}(\bar{\theta}) = \overline{\sigma_{\text{d}}(\theta)}$; $\Sigma(\bar{\theta}) = \overline{\Sigma(\theta)}$.

(d1) If $0 < \operatorname{Im} \theta < \min\{\alpha, \frac{1}{2}\pi\}$, then

$$\Sigma(\theta) \subset \mathbb{R} \cup \{\Sigma_{\min} + \mu \,|\, -2 \operatorname{Im} \theta < \arg \mu < 0\}$$

and $\mathbb{R} \cap \Sigma(\theta) = \Sigma(0)$. Moreover, if $0 < \operatorname{Im} \varphi < \operatorname{Im} \theta < \frac{1}{2}\pi$, then $\Sigma(\varphi) \subset \Sigma(\theta)$.

(d2) If $0 < \operatorname{Im} \theta < \frac{1}{2}\pi$, then $\sigma_{\text{d}}(\theta) \subset \mathbb{R} \cup \{\Sigma_{\min} + \mu \,|\, -2 \operatorname{Im} \theta < \arg \mu < 0\}$ and $\mathbb{R} \cap \sigma_{\text{d}}(\theta) = \sigma_{\text{pp}}(H) \backslash \Sigma(0)$. Moreover, if $0 < \operatorname{Im} \varphi < \operatorname{Im} \theta < \frac{1}{2}\pi$, then $\sigma_{\text{d}}(\varphi) \subset \sigma_{\text{d}}(\theta)$.

(e) $\sigma_{\text{sing}}(H) = \varnothing$.

Proof Since the proof directly follows that of Theorem XIII.36, we leave the details to the reader (Problems 78, 79). (a) and (c) follow from $U(\varphi)H(\theta)U(\varphi)^{-1} = H(\theta + \varphi)$ and $H(\bar{\theta}) = H(\theta)^*$, and the containment $\sigma_{\text{ess}}(\theta) \subset \{\mu + e^{-2\theta}\lambda \,|\, \mu \in \Sigma(\theta), \lambda \in [0, \infty)\}$ follows from Proposition 2. The containment $\{\mu + e^{-2\theta}\lambda \,|\, \mu \in \Sigma(\theta), \lambda \in [0, \infty)\} \subset \sigma_{\text{ess}}(\theta)$ requires a separate argument (Problem 78). (d1) for N-body systems follows from (d2) for $(N-1)$-body systems so only (d2) need be proven. This is accomplished, as

in Theorem XIII.36 in two parts. First, one uses the perturbation theory of discrete spectrum to show that $\sigma_d(\theta)$ is locally constant and uses this to prove all of (d2) but $[\Sigma_{min}, \infty) \cap \sigma_d(\theta) = \sigma_{pp}(H) \backslash (\Sigma(0) \cup (-\infty, \Sigma_{min}))$. This last fact is proven by analytic continuation of matrix elements $(\psi, (H - z)^{-1}\psi)$ for $\psi \in N_\alpha$. (e) follows as a by-product of this last development. ∎

Corollary An N-body quantum Hamiltonian with center of mass motion removed and with Coulomb or Yukawa potentials has an empty continuous singular spectrum.

Eigenvalues of $H(\theta)$ in $\sigma_d(\theta) \backslash \sigma_d(0)$ are called **resonance eigenvalues** of H. We have already discussed their significance in Section XII.6. Points in $\Sigma(\theta) \backslash \Sigma$ are called **complex thresholds** or **resonance thresholds**.

XIII.11 Properties of eigenfunctions

With the exception of the question of proving that $\sigma_{pp} = \sigma_{disc}$ (which we turn to in Section 13), we have completed our analysis of the different kinds of spectra of Schrödinger operators on infinite space with two body potentials going to zero at ∞. We turn now to a set of problems that are not spectral analysis per se but which are closely related. In this section we concentrate on regularity properties and falloff of eigenfunctions. There is a close connection between these two sets of properties for as we have seen (see Sections IX.2, 3) smoothness of a function ψ is closely connected to decrease properties of the Fourier transform $\hat{\psi}$. We shall state all our theorems below in terms of $\psi(x)$, the "x-space function," but in proofs $\hat{\psi}(p)$, "the p-space function" will often enter. We first discuss smoothness of $\psi(x)$, then the falloff of ψ in the sense that $\psi \in D(\exp(a|x|))$ in certain circumstances. Finally, we combine the two sets of ideas to prove pointwise bounds $|\psi(x)| \leq C \exp(-a|x|)$.

To state our smoothness results we introduce spaces of **uniformly Hölder continuous functions**:

Definition Let $0 < \theta < 1$. Then we say $f \in C_\theta(\mathbb{R}^n)$ if f: $\mathbb{R}^n \to \mathbb{C}$ is bounded and obeys

$$|f(x) - f(y)| \leq C|x - y|^\theta$$

for some fixed C and all $x, y \in \mathbb{R}^n$. We set

$$\|f\|_{(\theta)} \equiv \|f\|_\infty + \sup_{x \neq y} |x-y|^{-\theta} |f(x) - f(y)|$$

We say $f \in C^1_\theta(\mathbb{R}^n)$ if f is bounded, C^1, and for each $j = 1, \ldots, n$, $\partial f/\partial x_j \in C_\theta(\mathbb{R}^n)$. We set

$$\|f\|_{\theta,1} = \|f\|_\infty + \sum_{j=1}^n \|D_j f\|_{(\theta)}$$

The connection of Hölder continuity and the Fourier transform is illustrated by:

Lemma 1 Let $(1+k^2)^{\beta/2}\hat{f}(k) \in L^1(\mathbb{R}^n)$. Then:

(a) If $0 < \beta < 1$, then $f \in C_\beta$ and

$$\|f\|_{(\beta)} \leq c\|(1+k^2)^{\beta/2}\hat{f}(\cdot)\|_1$$

(b) If $1 < \beta < 2$, then $f \in C^1_{\beta-1}$ and

$$\|f\|_{\beta-1,1} \leq c_n \|(1+k^2)^{\beta/2}\hat{f}\|_1$$

Proof (a) For each real s, $|e^{is}-1| \leq 2$ and $|e^{is}-1| \leq \left|\int_0^s e^{it}\,dt\right| \leq s$, so $|e^{is}-1| \leq s^\beta 2^{1-\beta}$. Thus

$$\begin{aligned} |e^{ik\cdot x} - e^{ik\cdot y}| &= |e^{ik\cdot(x-y)} - 1| \\ &\leq 2^{1-\beta}|k|^\beta |x-y|^\beta \end{aligned}$$

so that

$$\begin{aligned} |f(x) - f(y)| &\leq (2\pi)^{-n/2} \int |\hat{f}(k)|\,|e^{ik\cdot x} - e^{ik\cdot y}|\,dk \\ &\leq \left[2^{1-\beta}(2\pi)^{-n/2} \int |\hat{f}(k)|\,|k|^\beta\,dk\right] |x-y|^\beta \\ &\leq 2^{1-\beta}(2\pi)^{-n/2}\|(1+k^2)^{\beta/2}\hat{f}\|_1\,|x-y|^\beta \end{aligned}$$

Since $\|f\|_\infty \leq \|f\|_1$, (a) follows.

The proof of (b) is similar to (a) and is left to the reader (Problem 80). ∎

We can now see what sort of smoothness result to expect by considering $H = -\Delta + V$ on $\mathbb{R}^3$ when $V \in L^2 + L^\infty$. Then $D(H) = D(-\Delta)$ by Kato's theorem. But if $\psi \in D(-\Delta)$, then $(1+k^2)\hat{\psi} \in L^2$ so for any $\beta < \frac{1}{2}$, $(1+k^2)^{\beta/2}\hat{\psi} \in L^1$ since $(1+k^2)^{-(1-\beta/2)}$ is then in $L^2(\mathbb{R}^3)$. We conclude that

$D(H) \subset C_\theta$ if $\theta < \frac{1}{2}$. For N-body Hamiltonians with two-body potentials, it is reasonable to expect that eigenfunctions should have no worse singularities than those produced by the two-body potentials in the two-body case. To state a sharp result, we introduce a special class of potentials.

Definition Let n be given and suppose $\sigma \geq 1$ and $\sigma > \frac{1}{2}n$. We say that a real-valued measurable function V on $\mathbb{R}^n$ is in class $M_\sigma^{(n)}$ if and only if

$$\hat{V} \in L^{\sigma'} + L^1$$

where $\sigma' = (1 - \sigma^{-1})^{-1}$ is the dual index to σ.

Example 1 Let $V(r) = |r|^{-1}$ on $\mathbb{R}^3$ be the Coulomb potential. Then $\hat{V}(k) = c|k|^{-2} \in L^{\sigma'} + L^1$ if $\sigma' > \frac{3}{2}$ so $V \in M_\sigma^{(3)}$ if $\sigma < 3$. The same conclusion holds for the Yukawa potential $V(r) = e^{-\mu|r|}/|r|$.

Proposition

(a) If $\sigma \geq 2$ and $\sigma > \frac{1}{2}n$ and if $V \in M_\sigma^{(n)}$, then V is $-\Delta$-bounded with relative bound zero.

(b) If $\sigma \geq 1$ and $\sigma > \frac{1}{2}n$ and if $V \in M_\sigma^{(n)}$, then V is $-\Delta$ form-bounded with relative bound zero.

Proof (a) By the Plancherel theorem, we need only prove that $\|(p^2 + a)^{-1}\hat{V} * \psi\|_2 \leq C_a \|\psi\|_2$ for all $\psi \in L^2$ where C_a is independent of ψ and can be chosen arbitrarily small by making a large. This follows from Young's and Hölder's inequalities. The proof of (b) is similar. ∎

The following theorem gives regularity properties of eigenfunctions since any eigenfunction of $\tilde{H}$ is clearly in $C^\infty(\tilde{H})$. Since $C^\infty(\tilde{H})$ is left invariant by $e^{-it\tilde{H}}$, it also implies regularity properties of solutions of the time-dependent Schrödinger equation with sufficiently regular initial data.

Theorem XIII.38 (the Kato–Simon theorem) Let

$$\tilde{H} = -\sum_{i=1}^{N} (2\mu_i)^{-1}\Delta_i + \sum_{i<j} V_{ij}(r_i - r_j)$$

as an operator on $L^2(\mathbb{R}^{Nn})$ where a point in $\mathbb{R}^{Nn}$ is written $\langle r_1, \ldots, r_N \rangle$ with $r_i \in \mathbb{R}^n$. Suppose that $\sigma \geq 1$, $\sigma > \frac{1}{2}n$ and that each V_{ij} is in $M_\sigma^{(n)}$. Then:

(a) If $\psi \in C^\infty(\tilde{H})$, then $\psi \in C_\theta$ for any $\theta < \min\{1, 2 - \sigma^{-1}n\}$.
(b) If $\sigma > n$, and $\psi \in C^\infty(\tilde{H})$, then $\psi \in C_\theta^1$ for any $\theta < 1 - \sigma^{-1}n$.

Moreover, the embeddings are continuous in the sense that given θ, there exist m and C with $\|\psi\|_{(\theta)} \leq C[\|\tilde{H}^m\psi\| + \|\psi\|]$ for all $\psi \in C^\infty(\tilde{H})$. Identical results hold if $\tilde{H}$ is replaced with H, the operator on $L^2(\mathbb{R}^{(N-1)n})$, obtained by removing the center of mass motion from $\tilde{H}$.

Proof We consider only the case where $\sigma \geq 2$, thus avoiding the need for quadratic form techniques. The general $\sigma \geq 1$ case is discussed in the reference quoted in the Notes. We also leave it to the reader to prove that the embeddings are continuous (Problem 82).

Let $H_0 = -\sum_{i=1}^{N} (2\mu_i)^{-1}\Delta_i$ and let $t_0(k)$ be the function $\sum_{i=1}^{N} (2\mu_i)^{-1}k_i^2$ on $\mathbb{R}^{Nn}$. We first claim that

$$\|(t_0(k) + 1)^{-\beta}\hat{V}_{ij} * \eta\|_p \leq C\|\eta\|_p \tag{66}$$

for any $p \in [1, 2]$, $\eta \in L^p(\mathbb{R}^{Nn})$, and β with $\beta > (2\sigma)^{-1}n$. In (66), C is independent of η and p (it is dependent only on V_{ij}, t_0, and β) and $\hat{V}_{ij}$is the Fourier transform in all Nn variables; thus

$$\begin{aligned}(\hat{V}_{ij} * \eta)(k_1, \ldots, k_N) \\ = \int (2\pi)^{(Nn-n)/2} f(\ell)\eta(k_1, \ldots, k_i - \ell, \ldots, k_j + \ell, \ldots, k_N)\, d^n\ell\end{aligned}$$

where f is the $\mathbb{R}^n$ Fourier transform of V_{ij}. To prove (66) we first notice that since $p \leq 2$ and $\sigma \geq 2$, Hölder's and Young's inequalities imply that

$$\|(k^2 + 1)^{-\beta} f * \varphi\|_p \leq C_2\|\varphi\|_p \tag{67}$$

if $\varphi \in L^p(\mathbb{R}^n)$ since $\beta > (2\sigma)^{-1}n$ tells us that $(k^2 + 1)^{-\beta} \in L^\sigma$. From (67) we immediately conclude that

$$\|[(k_i - k_j)^2 + 1]^{-\beta}\hat{V}_{ij} * \eta\|_p \leq C_1\|\eta\|_p$$

for all $\eta \in L^p(\mathbb{R}^{Nn})$ by raising both sides of (67) to the pth power and integrating over dummy variables. Since $[(k_i - k_j)^2 + 1]^\beta[t_0(k) + 1]^{-\beta}$ is bounded, (66) holds.

Next suppose that $p \in [1, 2]$, $\beta > (2\sigma)^{-1}n$, and we know that $\psi \in D(\tilde{H})$ with $\hat{\psi}$ and $\mathscr{F}(\tilde{H}\psi)$ in L^p. Then we claim that $(t_0(k) + 1)^{(1-\beta)}\hat{\psi} \in L^p$. For we can write

$$\begin{aligned}\hat{\psi} &= \mathscr{F}[(H_0 + I)^{-1}(\tilde{H} + I - V)\psi] \\ &= (t_0(k) + 1)^{-1}(\mathscr{F}(\tilde{H}\psi) + \hat{\psi}) - (2\pi)^{-Nn/2}(t_0(k) + 1)^{-1}\sum_{i<j}\hat{V}_{ij} * \hat{\psi}\end{aligned}$$

so that (66) implies that $(t_0(k) + 1)^{(1-\beta)}\hat{\psi} \in L^p$.

Now we can complete the proof. Since $\sigma > \frac{1}{2}n$, choose β so that $(2\sigma)^{-1}n < \beta < 1$. Suppose that $\psi \in C^\infty(\tilde{H})$. Then by the above,

$$(k^2 + 1)^{1-\beta}\mathscr{F}(\tilde{H}^m\psi) \in L^2$$

for all m. Since $(k^2 + 1)^{-(1-\beta)} \in L^r$ for all $r \in (r_0, \infty)$ and some $r_0 < \infty$, we conclude that $\mathscr{F}(\tilde{H}^m\psi) \in L^q$ as long as $q^{-1} - r_0^{-1} < \frac{1}{2}$ and $q \geq 1$. By repeating this argument j times we see that $\mathscr{F}(\tilde{H}^m\psi) \in L^q$ as long as $q^{-1} - jr_0^{-1} < \frac{1}{2}$. Choosing j suitably, we conclude that $\mathscr{F}(\tilde{H}\psi)$ and $\hat{\psi}$ are in L^1. Invoking the argument in the preceding paragraph once more we see that $(k^2 + 1)^{1-\beta}\hat{\psi} \in L^1$ so long as $\beta > (2\sigma)^{-1}n$ and $\psi \in C^\infty(\tilde{H})$. Lemma 1 now completes the proof. ∎

Corollary Let H be an atomic Hamiltonian. Then any $\psi \in C^\infty(H)$ is a C^∞ function on $\mathbb{R}^{3N-3}\backslash\{\langle r_1, \ldots, r_{N-1}\rangle \mid \text{some } r_i = 0 \text{ or some } r_i = r_j\}$ and is uniformly Hölder continuous of order θ for any $\theta < 1$ on all of $\mathbb{R}^{3N-3}$.

Proof The first statement follows from the technique of the elliptic regularity theorem (Problem 83); the second from Theorem XIII.38. ∎

* * *

The second topic we discuss in this section is that of the exponential falloff of eigenfunctions in the discrete spectrum. We first present L^2 results in various forms and then pointwise bounds. We begin with an L^2 result which is easy to prove and later give a sharper L^2 result which requires some kinematical preliminaries.

Theorem XIII.39 Let $\tilde{H} = -\sum_{i=1}^{N}(2\mu_i)^{-1}\Delta_i + \sum_{i<j} V_{ij}(r_i - r_j)$ on $L^2(\mathbb{R}^{3N})$ and let H be the operator on $L^2(\mathbb{R}^{3N-3})$ obtained by removing the center of mass motion from $\tilde{H}$. Suppose that each V_{ij} is a form-bounded perturbation of $-\Delta$ on $\mathbb{R}^3$ with relative bound 0. Let $E \in \sigma_{\text{disc}}(H)$ and let $H\psi = E\psi$. Then $\psi \in D(e^{ar})$ for some $a > 0$ where $r = (\sum_{j=1}^{3N-3} x_j^2)^{1/2}$ in terms of some set of coordinates for $\mathbb{R}^{3N-3}$.

Proof Since

$$e^{ar} \leq \exp(a\sqrt{3N-3}\,\max|x_j|) \leq \sum_{j=1}^{3N-3}\exp(a|x_j|\sqrt{3N-3})$$

we need only show that ψ is an analytic vector for each position operator x_j. We can write $H = H_0 + V$ with $H_0 = t(p)$ where $t(v) = \sum_{i<j} a_{ij}v_iv_j$ and p is the $(3N-3)$-tuple of operators with $p_j = -i\,\partial/\partial x_j$ and $\{a_{ij}\}$ is positive definite.

The idea is to employ the dilation analytic techniques of Section 10 but with a different group. Fix j and let $W(\alpha) = e^{i\alpha x_j}$. Then

$$H_0(\alpha) \equiv W(\alpha) H_0 W(\alpha)^{-1} = t(p_1, \ldots, p_j - \alpha, \ldots, p_{3N-3})$$

and

$$V(\alpha) \equiv W(\alpha) V W(\alpha)^{-1} = V$$

Thus both $H_0(\alpha)$ and $V(\alpha)$ have analytic continuations to the entire α plane. Moreover, it is easy to see that for each fixed α, $\frac{1}{2}H_0 \leq \text{Re } H_0(\alpha) + c_\alpha$ where c_α is an α-dependent constant. It follows that $H(\alpha) \equiv H_0(\alpha) + V(\alpha)$ is an entire analytic family of type (B).

The theory of Section XII.2 is therefore applicable, so there is an a and functions $f_1, \ldots, f_k$ in $\{\alpha \,|\, |\alpha| < a\}$ with at worst algebraic singularities at $\alpha = 0$ so that the branches of $f_1(\alpha), \ldots, f_k(\alpha)$ are all the eigenvalues of $H(\alpha)$ near E. Moreover, there exists a projection valued analytic function $P(\alpha)$ on $\{\alpha \,|\, |\alpha| < a\}$ so that Ran $P(\alpha)$ is the set of eigenvectors for $H(\alpha)$ with eigenvalues $f_1(\alpha), \ldots, f_k(\alpha)$. Now, for α real, $H(\alpha) = W(\alpha) H W(\alpha)^{-1}$ so for such α, $f_1(\alpha) = \cdots = f_k(\alpha) = E$ and $W(\alpha)P(0)W(\alpha)^{-1} = P(\alpha)$. It follows by analyticity that f_i is always equal to E and that

$$W(\alpha_0)P(\alpha)W(\alpha_0)^{-1} = P(\alpha + \alpha_0)$$

if α_0 is real and $|\alpha| < a$, $|\alpha + \alpha_0| < a$. The fact that ψ is an analytic vector for x_j now follows from the proposition below. ∎

Proposition (O'Connor's lemma) Let $W(\alpha) = e^{i\alpha A}$ be a one-parameter unitary group and let D be a connected region in $\mathbb{C}$ with $0 \in D$. Suppose that a projection-valued analytic function $P(\alpha)$ is given on D with $P(0)$ of finite rank so that

$$W(\alpha_0)P(\alpha)W(\alpha_0)^{-1} = P(\alpha + \alpha_0)$$

for all pairs $\langle \alpha, \alpha_0 \rangle$ with α_0 real and with $\alpha, \alpha + \alpha_0 \in D$. Let $\psi \in$ Ran $P(0)$. Then the function $\psi(\alpha) \equiv W(\alpha)\psi$ has an analytic continuation from $D \cap \mathbb{R}$ to D. In particular, ψ is an analytic vector for A.

Proof Let $\mathscr{A}_D$ denote the set of vectors φ for which $\varphi(\alpha) \equiv W(\alpha)\varphi$ has an analytic continuation from $D \cap \mathbb{R}$ to D. Then $\mathscr{A}_D$ is dense in the underlying Hilbert space (see Section X.6) so $P(0)[\mathscr{A}_D]$ is dense in Ran $P(0)$. Since Ran $P(0)$ is finite dimensional, $P(0)[\mathscr{A}_D] =$ Ran $P(0)$. Thus we need only prove that $P(0)[\mathscr{A}_D] \subset \mathscr{A}_D$. Let $\varphi \in \mathscr{A}_D$ and let $\eta(\alpha) = P(\alpha)\varphi(\alpha)$ for $\alpha \in D$. Clearly $\eta(\alpha)$ is analytic and for $\alpha \in D \cap \mathbb{R}$

$$\eta(\alpha) = P(\alpha)W(\alpha)\varphi = W(\alpha)(P(0)\varphi)$$

so $P(0)\varphi \in \mathscr{A}_D$. ∎

To obtain better results on how big the constant a in the statement $\psi \in D(e^{ar})$ can be, it is necessary to introduce some kinematics connected with the meaning of r.

Definition Given particles with masses $\mu_1, \ldots, \mu_N$ at points $\mathbf{r}_1, \ldots, \mathbf{r}_N$ we define the **total mass** $M = \sum \mu_i$, the **center of mass** $\mathbf{R} = M^{-1} \sum_{i=1}^{N} \mu_i \mathbf{r}_i$, and the **radius of gyration** $r = [M^{-1} \sum \mu_i (\mathbf{r}_i - \mathbf{R})^2]^{1/2}$.

Definition Given an N-body free quantum Hamiltonian $\tilde{H}_0$ on $L^2(\mathbb{R}^{3N})$, a set of coordinates $\zeta_1, \ldots, \zeta_{N-1}$ orthogonal to $\mathbf{R}$ is called a **set of normal coordinates** if and only if

$$\tilde{H}_0 = -(2M)^{-1} \left[\Delta_{\mathbf{R}} + \sum_{i=1}^{N} \Delta_{\zeta_i} \right]$$

To see that normal coordinates exist, pass first to a set of Jacobi coordinates, $\xi_1, \ldots, \xi_{N-1}$ so that

$$\tilde{H}_0 = (-2M)^{-1} \Delta_{\mathbf{R}} + \sum (-2M_j)^{-1} \Delta_{\xi_j}$$

and let $\zeta_j = (M_j/M)^{1/2} \xi_j$.

Proposition

(a) The radius of gyration r is a function of the coordinates orthogonal to $\mathbf{R}$.

(b) If $\zeta_1, \ldots, \zeta_{N-1}$ is a set of normal coordinates, then

$$r = \left(\sum_{i=1}^{N-1} |\zeta_i|^2 \right)^{1/2}$$

Proof We first notice that

$$Mr^2 + MR^2 = \sum_{i=1}^{N} \mu_i r_i^2$$

Let $\eta_i = (\mu_i/M)^{1/2} r_i$ so that

$$\tilde{H}_0 = -(2M)^{-1} \sum_{i=1}^{N} \Delta_{\eta_i} \tag{68a}$$

and

$$Mr^2 + MR^2 = M \sum_{i=1}^{N} \eta_i^2 \tag{68b}$$

By (68a), the coordinate change from $\langle \eta_1, \ldots, \eta_N \rangle$ to $\langle \mathbf{R}, \zeta_1, \ldots, \zeta_{N-1} \rangle$ is orthogonal if $\langle \zeta_1, \ldots, \zeta_{N-1} \rangle$ is a set of normal coordinates, and thus by (68b),

$$r^2 + R^2 = R^2 + \sum_{i=1}^{N-1} \zeta_i^2 \quad \blacksquare$$

Theorem XIII.40 (O'Connor–Combes–Thomas theorem) Let $\tilde{H} = \tilde{H}_0 + \sum_{i<j} V_{ij}(r_i - r_j)$ be an N-body Hamiltonian on $L^2(\mathbb{R}^{3N})$ with each $V_{ij} \in R + (L^\infty)_\varepsilon$. Let H be the operator on $L^2(\mathbb{R}^{3N-3})$ obtained from $\tilde{H}$ by removing the center of mass motion. Let $\Sigma = \inf \sigma_{\text{ess}}(H)$ and let ψ be an eigenfunction of H with eigenvalue $E < \Sigma$. Then $\psi \in D(e^{ar})$, where r is the radius of gyration, whenever $a^2 < 2M(\Sigma - E)$.

Proof We outline the proof and leave the details to the reader. Let $\zeta_1, \ldots, \zeta_{N-1}$ be a set of normal coordinates and define $W(\alpha) = \exp(i(\alpha_1 \cdot \zeta_1 + \cdots + \alpha_{N-1} \cdot \zeta_{N-1}))$ for $\alpha = \langle \alpha_1, \ldots, \alpha_{N-1} \rangle \in \mathbb{C}^{3N-3}$. Suppose we can prove that $\psi \in D(W(\alpha))$ if $|\alpha| \equiv (|\alpha_1|^2 + \cdots + |\alpha_{N-1}|^2)^{1/2} < \sqrt{2M(\Sigma - E)}$. Then a simple geometric argument (Problem 86a) shows that $\psi \in D(e^{ar})$ if $a < \sqrt{2M(\Sigma - E)}$.

It is thus sufficient to prove that $W(\alpha)\psi$ defined for $\alpha \in \mathbb{R}^{3N-3}$ has a continuation into the region $\{\alpha \,|\, |\text{Im } \alpha|^2 < 2M(\Sigma - E)\}$. Let

$$H_0(\alpha) = -(2M)^{-1} \sum_{i=1}^{N-1} (\nabla_{\zeta_i} - i\alpha_i)^2$$

and let $H(\alpha) = H_0(\alpha) + V$. Then, an analysis similar to that given in Section 10 (Problem 86b) shows that

$$\sigma_{\text{ess}}(H(\alpha)) = \bigcup_D \{\lambda + \mu \,|\, \lambda \in \Sigma_D(\alpha), \mu \in K_D\}$$

where $\Sigma_D(\alpha)$ are the thresholds associated with a cluster decomposition D and $K_D = \{t_D(p - \alpha) \,|\, p \in \mathbb{R}^{3N-3}\}$ where t_D is the kinetic energy between the clusters in D. By induction, it is easy to show (Problem 86c) that

$$\sigma_{\text{ess}}(H(\alpha)) \subset \{\lambda \,|\, \text{Re } \lambda \geq \Sigma - (2M)^{-1}(\text{Im } \alpha)^2\}$$

Thus if $(\text{Im } \alpha)^2 < \sqrt{2M(\Sigma - E)}$, E remains disjoint from $\sigma_{\text{ess}}(H(\alpha))$. Thus, by following the arguments of Section 10, E is an eigenvalue of $H(\alpha)$ for all such α. The proof is completed (Problem 86d) by mimicking the proof of Theorem XIII.39 and employing O'Connor's lemma. ∎

If the potentials are dilation analytic, one can also prove exponential falloff for eigenfunctions associated with eigenvalues in the continuum. This result will have applications in Section 13.

Theorem XIII.41 Let $\tilde{H} = \tilde{H}_0 + \sum_{i<j} V_{ij}$ where each multiplication operator V_{ij} is a dilation analytic potential in some $\mathscr{F}_\beta$. Let E be a non-threshold eigenvalue for H with eigenfunction ψ. Then:

(a) $\psi \in D(e^{ar})$ for some $a > 0$.
(b) If $U(\theta)$ is the family of dilations, and $\beta_0 = \min\{\beta, \frac{1}{2}\pi\}$, then $U(\theta)\psi \equiv \psi(\theta)$ has a continuation into the strip $\{\theta \,|\, |\operatorname{Im}\theta| < \beta_0\}$ and for each θ in the strip, $\psi(\theta) \in D(e^{ar})$ for some $a > 0$.
(c) If E is larger than the largest threshold, then the β_0 of (b) may be chosen to be $\min\{\beta, \pi\}$.
(d) If each V_{ij} has the property that $V_{ij}(\theta)$ has a continuation into the strip $\{\theta \,|\, |\operatorname{Im}\theta| \leq \beta\}$ analytic in the interior, continuous on the whole strip, and if $\beta < \frac{1}{2}\pi$ (or if E is larger than the largest threshold, if $\beta < \pi$), then $\psi(\theta)$ has a continuation to that strip, analytic in the interior, continuous on the whole strip, with $\psi(\theta) \in D(e^{ar})$ for some $a > 0$.

Proof By the analysis of Section 10, E is an eigenvalue of $H(\theta)$ for all θ in the strip $\{\theta \,|\, |\operatorname{Im}\theta| < \beta_0\}$; or in case (d), $\{\theta \,|\, |\operatorname{Im}\theta| \leq \beta_0\}$. Let $P(\theta)$ be the associated projection, defined as a spectral projection if θ is real and by the method of Section XII.2 if $\operatorname{Im}\theta \neq 0$. Clearly, $P(\theta)$ is analytic in the regions $\{\theta \,|\, 0 < |\operatorname{Im}\theta| < \beta_0\}$ and by the arguments in Section 10, $P(\theta)$ is continuous in $\{\theta \,|\, 0 \leq |\operatorname{Im}\theta| < \beta_0\}$. Moreover $P(\theta)$ is self-adjoint if θ is real. By the Schwartz reflection principle, $P(\theta)$ is analytic in the whole strip $\{\theta \,|\, |\operatorname{Im}\theta| < \beta_0\}$. The analyticity properties of $\psi(\theta)$ now follow from O'Connor's lemma.

If $\operatorname{Im}\theta \neq 0$, E is a discrete eigenvalue so we can prove that $\psi(\theta) \in D(e^{ar})$ for some $a > 0$ by following the proof of Theorem XIII.39. Let us suppose that $\psi(\theta_0) \in D(\exp(a_0 e^{\theta_0} r))$ with $|\operatorname{Im}\theta_0| < \frac{1}{4}\pi$. We will show that $\psi \in D(e^{a_0 r})$. Let $\varepsilon > 0$ be given, let $\eta \in L^2(\mathbb{R}^{3N-3})$, and define

$$F(\theta) = (\eta, \exp(-\varepsilon r^2 e^{2\theta})\exp(a_0 e^{\theta} r)\psi(\theta))$$

Clearly $F(\theta)$ is analytic in the strip $\{\theta \,|\, |\operatorname{Im}\theta| < |\operatorname{Im}\theta_0| + \delta\}$ for suitable δ. Moreover $F(\theta)$ is uniformly bounded on the strip and for $\operatorname{Im}\theta = \pm |\operatorname{Im}\theta_0|$, we have $|F(\theta)| \leq \|\eta\| \, \|\exp(a_0 e^{\theta_0} r)\psi(\theta_0)\|$. By the maximum principle, this last inequality holds for all θ; in particular

$$|(\eta, e^{-\varepsilon r^2} e^{a_0 r}\psi)| \leq C\|\eta\|$$

for all η and ε. It follows that $\psi \in D(\exp(a_0 r))$. ∎

As with Theorem XIII.39, Theorem XIII.41 has a sharp form where an estimate on a_0 is given (see the Notes).

We finally turn to proving pointwise exponential bounds:

Theorem XIII.42 Let H be an N-body Hamiltonian on $L^2(\mathbb{R}^{3N-3})$ with potentials in $M_\sigma^{(3)}$ for some $\sigma > \frac{3}{2}$. Suppose that $\psi \in C^\infty(H)$ and for some a and all n, $H^n\psi \in D(e^{ar})$ where r is the radius of gyration. Then, for each ε, there is a constant C_ε with

$$|\psi(\zeta)| \leq C_\varepsilon e^{-(a-\varepsilon)r}$$

for all ζ. In particular, if the hypotheses of Theorem XIII.40 hold and, in addition, each $V_{ij} \in M_\sigma^{(3)}$, then

$$|\psi(\zeta)| \leq C_a e^{-ar}$$

for any $a < \sqrt{2M(\Sigma - E)}$.

Proof The proof is an application of the Fourier transform, especially of the ideas behind the Paley–Wiener theorem. Pass to normal coordinates so that $r = (\sum_{i=1}^{N-1} |\zeta_i|^2)^{1/2}$. If $\varphi \in D(e^{ar})$, then for any $k \in \mathbb{C}^{3N-3}$ with $|\operatorname{Im} k| < a$, $\varphi_k \equiv e^{-ik\cdot\zeta}\varphi(\zeta)$ is in $L^1(\mathbb{R}^{3N-3})$ because $\exp(-br) \in L^2$ for any $b > 0$. Moreover, the map $k \mapsto \varphi_k$ is analytic in k as an L^1-valued function. Thus the function

$$\hat{\varphi}(k) = (2\pi)^{-(3N-3)/2} \int \varphi_k(\zeta)\, d\zeta$$

is analytic in the tube $\{k \,|\, |\operatorname{Im} k| < a\}$. By the Plancherel theorem, for any $b < a$, there is a constant C_b with

$$\int_{k \in \mathbb{R}^{3N-3}} |\hat{\varphi}(k + i\kappa)|^2 \, d^{3N-3}k < C_b \tag{69}$$

if $|\kappa| \leq b$. At this point, we follow the proof of Theorem XIII.38. By analytic continuation, $\hat{\varphi}(k)$ obeys the equation

$$(2M)^{-1}k^2\hat{\varphi}(k) + (2\pi)^{-(3N-3)/2} \int \hat{V}(\ell)\hat{\varphi}(k-\ell)\, d^{3N-3}\ell = \widehat{H\varphi}(k)$$

for all k with $|\operatorname{Im} k| < a$ whenever φ and $H\varphi$ are in $D(e^{ar})$. By following the proof of Theorem XIII.38 and using (69) one shows (Problem 88) that for any $b < a$, there is constant D_b with

$$\int |\hat{\psi}(k + i\kappa)|\, d^{3N-3}\kappa < D_b \tag{70}$$

if $|\kappa| \leq b$ and if $\psi, H\psi, \ldots, H^m\psi \in D(\exp(ar))$ for suitable m. Since $\hat{\psi}(\cdot + i\kappa)$ is the Fourier transform of $e^{\kappa \cdot \zeta}\psi(\zeta)$, (70) implies that

$$|e^{\kappa \cdot \zeta}\psi(\zeta)| \leq D_b(2\pi)^{-(3N-3)/2}$$

if $|\kappa| \leq b$. Taking a sup over such κ we see that

$$|e^{br}\psi(\zeta)| \leq D_b(2\pi)^{-(3N-3)/2} \quad \blacksquare$$

Corollary Let H be an atomic Hamiltonian. Then any eigenfunction ψ corresponding to a point in the discrete spectrum obeys an estimate of the form

$$|\psi(\zeta)| \leq C_a e^{-ar}$$

for some positive a.

XIII.12 Nondegeneracy of the ground state

Our main result in this section will concern a self-adjoint operator H that is bounded below and has an eigenvalue as the lowest point in its spectrum. Under certain conditions, we shall show that the eigenspace corresponding to that eigenvalue is one dimensional and that the corresponding eigenvector is a strictly positive function in a particular realization of the underlying Hilbert space as an L^2 space. The eigenvalue is called the **ground state energy** and the eigenvector the **ground state**. As is the case with so much spectral analysis, the method of verifying the conditions in applications is a perturbative technique. At first sight this is surprising since we shall be interested in Schrödinger operators and $H_0 = -\Delta$ does not possess any eigenfunctions! It will thus be important that all our results will be in terms of conclusions of the form: "Either H has no eigenvalue below the essential spectrum or it has a nondegenerate ground state energy with associated eigenvector strictly positive." Finally, we note that, as usual, it is easier to study the bounded operators e^{-itH} and $(H+1)^{-1}$ rather than H. If E_0 is the ground state energy for H, then e^{-itE_0} is the *largest* eigenvalue of e^{-itH}. We begin by studying a bounded operator A and its largest eigenvalue.

Definition Let $\langle M, \mu\rangle$ be a σ-finite measure space. $f \in L^2(M, d\mu)$ is called **positive** if f is nonnegative a.e. and is not the zero function. f is called **strictly positive** if $f(x) > 0$ a.e.. A bounded operator A on L^2 is called **positivity preserving** if Af is positive whenever f is positive. A is called **positivity**

improving if Af is strictly positive whenever f is positive. Finally, A is called **ergodic** if and only if it is positivity preserving and for any $u, v \in L^2$ that are both positive there is some $n > 0$ for which $(u, A^n v) \neq 0$.

We remark that by definition the zero function is not positive; so if A is positivity preserving, then Af is not the zero function for any positive function f. Moreover, by the following reformulation, every positivity improving map is ergodic: A function $g \in L^2(M, d\mu)$ is strictly positive if and only if $(f, g) > 0$ for all positive functions f. Thus, a bounded operator A on $L^2(M, d\mu)$ is positivity improving if and only if $(u, Av) > 0$ for all positive functions $u, v \in L^2(M, d\mu)$.

Example 1 Let $A = (-\Delta + 1)^{-1}$ on $L^2(\mathbb{R}^3)$. Equation (IX.30) states that

$$(f, Ag) = \int \overline{f(x)} g(y) \frac{e^{-|x-y|}}{4\pi|x-y|} d^3x\, d^3y$$

Since $(4\pi|x-y|)^{-1} e^{-|x-y|}$ is strictly positive, A is positivity improving. Similarly, the explicit formula for $e^{t\Delta}$ on $L^2(\mathbb{R}^n)$ shows that it is also positivity improving.

Example 2 Let $\langle M, \mu \rangle$ be a probability measure space, i.e., $\mu(M) = 1$ and let $T: M \to M$ be a measure preserving map. Let $(Af)(x) = f(Tx)$. A is a unitary operator that is clearly positive preserving. It is never positivity improving. A is ergodic if and only if T is ergodic in the sense defined in Section II.5 (Problem 90).

Example 3 (second quantized operators on a Fock space) We saw in the proof of Theorem X.61 (Section X.9) that $\Gamma(e^{-tA})$ is positivity preserving as an operator on Q space whenever A is a positive self-adjoint operator on the one-particle space that commutes with the distinguished complex conjugation. We shall examine later the question of when it is ergodic or positivity improving.

The main abstract theorem of this section is the following:

Theorem XIII.43 Let A be a bounded, positive operator on $L^2(M, d\mu)$. Suppose that A is positivity preserving and that $\|A\|$ is an eigenvalue. Then the following are equivalent:

(a) $\|A\|$ is a simple eigenvalue and the associated eigenvector is strictly positive.

(b) A is ergodic.
(c) $L^\infty(M) \cup \{A\}$ acts irreducibly, i.e., no nontrivial closed subspace is left invariant by both A and every bounded multiplication operator.

Proof We prove (a) $\Rightarrow$ (b) $\Rightarrow$ (c) $\Rightarrow$ (a).

(a) $\Rightarrow$ (b) Let $B = A/\|A\|$ and let $\{P_\Omega\}$ be the spectral projections for B. Since $x^n \to 0$ if $0 \leq x < 1$ and $x^n \to 1$ if $x = 1$, the functional calculus implies that

$$\operatorname*{s-lim}_{n\to\infty} B^n = P_{\{1\}}$$

By hypothesis, $P_{\{1\}} = (\psi, \cdot)\psi$ where ψ is strictly positive. Thus for any positive u, v,

$$\lim_{n\to\infty} (u, B^n v) = (u, \psi)(\psi, v) > 0$$

As a result, for some n, $(u, A^n v) = \|A\|^n (u, B^n v) > 0$.

(b) $\Rightarrow$ (c) Suppose (c) does not hold. Let S be a nontrivial subspace left invariant by $L^\infty(M) \cup \{A\}$. Let $f \in S$ and let $h = \bar{f}/|f| \in L^\infty(M)$. Then $|f| = hf \in S$. Similarly, if $g \in S^\perp$, then $|g| \in S^\perp$. Choose $f \in S$, $g \in S^\perp$, $f \neq 0 \neq g$. Since A leaves S invariant, $A^n|f| \in S$, so

$$(|g|, A^n|f|) = 0$$

for all n. Thus A is not ergodic.

(c) $\Rightarrow$ (a) By hypothesis, $\|A\|$ is an eigenvalue. Let ψ be an eigenvector of A with eigenvalue $\|A\|$ and suppose that ψ is real valued. Since $|\psi| \pm \psi \geq 0$, we know that $A(|\psi| \pm \psi) \geq 0$ so

$$|A\psi| \leq A|\psi|$$

Thus

$$(|\psi|, A|\psi|) \geq (|\psi|, |A\psi|) \geq (\psi, A\psi) = \|A\| \, \|\psi\|^2$$

As a result, $A|\psi| = \|A\| \, |\psi|$ so $|\psi|$ is also an eigenvector. We shall show that $|\psi|$ is strictly positive. Let $S = \{f \in L^2(M, d\mu) \mid f\psi = 0 \text{ a.e.}\}$. S is clearly a subspace and moreover it is left invariant by $L^\infty(M)$. Let $S_+ = \{g \in S \mid g \geq 0\}$. Then for $f \in S_+$, $(Af, |\psi|) = (f, A|\psi|) = \|A\|(f, |\psi|) = 0$. Since Af is positive, $(Af)\psi = 0$ a.e., that is, $Af \in S_+$. Thus, A leaves S_+ invariant. Since $S = S_+ - S_+ + i(S_+ - S_+)$, A leaves S invariant. Thus by hypothesis (c), $S = \{0\}$ or $S = \mathscr{H}$. Since $\psi \notin S$ and $\psi \neq 0$, $S = \{0\}$, from which it follows that $|\psi| > 0$ a.e.

Thus we know that any real eigenvector with eigenvalue $\|A\|$ is nonzero a.e. and that also $A|\psi| = \|A\| \, |\psi|$. Thus $|\psi| - \psi$ is either an eigenvector with eigenvalue $\|A\|$ or it is identically 0 so that $|\psi| - \psi$ is either almost

everywhere vanishing or almost everywhere nonvanishing. This means that every real eigenvector with eigenvalue $\|A\|$ is a.e. strictly positive or a.e. strictly negative. If A had two real eigenvectors with eigenvalue $\|A\|$, it would have two orthogonal eigenvectors which were both a.e. positive. Since this is impossible, we conclude that A has only one real eigenvector of eigenvalue $\|A\|$ and that this eigenvector is strictly positive.

Finally, let ψ be an arbitrary eigenvector with eigenvalue $\|A\|$. Since A takes positive functions into positive functions, it takes real functions into real functions, so that $\mathrm{Re}(A\psi) = A(\mathrm{Re}\ \psi)$. Thus $\mathrm{Re}\ \psi$ and $\mathrm{Im}\ \psi$ are eigenvectors with eigenvalue $\|A\|$. It follows that ψ is a complex multiple of the unique real eigenvector. ∎

To apply this to the lowest eigenvalue of a self-adjoint operator, we can use either the resolvent or the semigroup generated by the operator. We first note:

Proposition Let H be a self-adjoint operator that is bounded from below. Let $E = \inf \sigma(H)$. Then e^{-tH} is positivity preserving for *all* $t > 0$ if and only if $(H - \lambda)^{-1}$ is positivity preserving for *all* $\lambda < E$.

Proof The proposition follows from the formulas

$$(H - \lambda)^{-1}\varphi = \int_0^\infty e^{\lambda t} e^{-Ht}\varphi \, dt \qquad (\lambda < E)$$

$$e^{-tH}\varphi = \lim_{n\to\infty} \left(1 + \frac{tH}{n}\right)^{-n} \varphi \qquad (t > 0) \tag{71}$$

These formulas, which are familiar from the theory of semigroups, (Section X.8) can be proven easily in the self-adjoint case by the functional calculus.

Theorem XIII.44 Let H be a self-adjoint operator that is bounded from below on $L^2(M, d\mu)$. Suppose that e^{-tH} is positivity preserving for all $t > 0$ and that $E = \inf \sigma(H)$ is an eigenvalue. Then the following are equivalent:

(a) E is a simple eigenvalue with a strictly positive eigenvector.
(b) $(H - \lambda)^{-1}$ is ergodic for some $\lambda < E$.
(c) e^{-tH} is ergodic for some $t > 0$.
(d) $(H - \lambda)^{-1}$ is positivity improving for all $\lambda < E$.
(e) e^{-tH} is positivity improving for all $t > 0$.

Proof By Theorem XIII.43, (a), (b), (c) are equivalent and clearly (d) ⇒ (b) and (e) ⇒ (c). We complete the proof by showing that (c) ⇒ (d) and (e).

$(c) \Rightarrow (d)$ Let u and v be positive. Since some e^{-tH} is ergodic, $(u, e^{-sH}v) > 0$ for some $s > 0$. But $(u, e^{-sH}v)$ is continuous so $(u, e^{-sH}v) > 0$ for s in some interval. Thus

$$(u, (H - \lambda)^{-1}v) = \int_0^\infty e^{\lambda s}(u, e^{-sH}v)\, ds > 0$$

$(c) \Rightarrow (e)$ Let u, v be positive and let $B = \{t > 0 \,|\, (u, e^{-tH}v) > 0\}$. Since B is nonempty and $(u, e^{-tH}v)$ is analytic in a neighborhood of the positive real axis, $(0, \infty)\backslash B$ can have only 0 as a limit point. In particular B contains arbitrarily small numbers. Thus, if we can show that $t > s$ and $s \in B$ implies $t \in B$, we can conclude that $B = (0, \infty)$. Fix $s \in B$. Then $(u, e^{-sH}v) > 0$ so that $u(\cdot)(e^{-sH}v)(\cdot)$ is not identically zero. Let $w = \min\{u, e^{-sH}v\}$. Then $w(m)$ is not identically zero. Since $e^{-\tau H}$ is positivity preserving,

$$\begin{aligned}(u, e^{-\tau H}(e^{-sH}v)) &\geq (u, e^{-\tau H}w) = (e^{-\tau H}u, w) \\ &\geq (e^{-\tau H}w, w) = \|e^{-\tau H/2}w\|^2 > 0\end{aligned}$$

We have used the fact that w is positive and that $e^{-\tau H/2}$ is positivity preserving to conclude that $e^{-\tau H/2}w \neq 0$. Thus $s \in B$ and $\tau > 0$ imply $s + \tau \in B$. ∎

Example 3, revisited Let A be an operator on a complex Hilbert space $\mathscr{H}$ that commutes with a distinguished complex conjugation and which obeys $A \geq cI$ for some $c > 0$. Let $H = d\Gamma(A)$ be the second quantization of A on $\mathscr{F}_s(\mathscr{H})$ thought of as an operator on $L^2(Q, d\mu)$ (see Section X.7). Then $H\Omega_0 = 0$ while $A \restriction \{\Omega_0\}^\perp \geq cI$. Thus H has a nondegenerate strictly positive ground state. We conclude that $\Gamma(e^{-tA}) = e^{-tH}$ is positivity improving for all $t > 0$.

In applications of Theorem XIII.44, the following perturbation theorem is very useful. There is another perturbation result based on the resolvent rather than the semigroup which is also useful (see Problems 91, 92).

Theorem XIII.45 Let H and H_0 be semibounded, self-adjoint operators on $L^2(M, d\mu)$ where $\langle M, \mu\rangle$ is a σ-finite measure space. Suppose that there exists a sequence of bounded multiplication operators V_n so that $H_0 + V_n$ converges to H in strong resolvent sense and so that $H - V_n$ converges to H_0 in strong resolvent sense. Suppose, moreover, that $H - V_n$ and $H_0 + V_n$ are uniformly bounded from below. Then:

(a) e^{-tH} is positivity preserving if and only if e^{-tH_0} is positivity preserving.
(b) $\{e^{-tH}\} \cup L^\infty(M, d\mu)$ acts irreducibly on $L^2(M, d\mu)$ if and only if $\{e^{-tH_0}\} \cup L^\infty(M, d\mu)$ acts irreducibly on $L^2(M, d\mu)$.

Proof By the Trotter product formula (Theorem VIII.31) and the continuity of the functional calculus (Theorem VIII.20),

$$e^{-tH} = \text{s-}\lim_{n\to\infty}\left(\text{s-}\lim_{m\to\infty}\left[e^{-tH_0/m}e^{-tV_n/m}\right]^m\right) \tag{72a}$$

$$e^{-tH_0} = \text{s-}\lim_{n\to\infty}\left(\text{s-}\lim_{m\to\infty}\left[e^{-tH/m}e^{+tV_n/m}\right]^m\right) \tag{72b}$$

Since $e^{\pm tV_n/m}$ is positivity preserving, we see that (a) holds. Moreover, (72) and the fact that $e^{\pm tV_n/m} \in L^\infty(M)$ imply that any subspace left invariant by e^{-tH_0} and $L^\infty(M)$ is left invariant by e^{-tH}. ∎

We can now apply Theorem XIII.44 to Schrödinger operators and to spatially cut-off $P(\varphi)_2$ Hamiltonians.

Theorem XIII.46 Let H be the Hamiltonian of an N-body Schrödinger system with center of mass motion removed. Suppose that the potentials V_{ij} are in $R + (L^\infty)_\varepsilon$. Then, if H has an eigenvalue at the bottom of its spectrum, the eigenvalue is nondegenerate and the corresponding eigenfunction is strictly positive.

Proof By Theorems XIII.43 and XIII.44, we need only prove that e^{-tH} is positivity preserving and that $\{e^{-tH}\} \cup L^\infty(\mathbb{R}^{3N-3})$ acts irreducibly. By Example 1 and the proof (b) ⇒ (c) in Theorem XIII.43, we know these facts for e^{-tH_0}. Let $V_{ij}^{(n)}$ be defined by

$$V_{ij}^{(n)}(x) = \begin{cases} V_{ij}(x) & \text{if } |V_{ij}(x)| \le n \\ n & \text{if } V_{ij}(x) > n \\ -n & \text{if } V_{ij}(x) < -n \end{cases}$$

It is easy to prove that $V_{ij} - V_{ij}^{(n)} \to 0$ in the Rollnik norm. By Theorem VIII.25c, $H_0 + \sum V_{ij}^{(n)} \to H$ and $H - \sum V_{ij}^{(n)} \to H_0$ in norm resolvent sense. Thus, Theorem XIII.45 is applicable and the proof is completed. ∎

Corollary Let H satisfy the hypothesis of Theorem XIII.46 and suppose that $H\psi = E\psi$ where $E = \inf \sigma(H)$. Let U be any positivity preserving unitary operator commuting with H. Then $U\psi = \psi$.

Proof Since U commutes with H, $H(U\psi) = E(U\psi)$. But E is nondegenerate so $U\psi = \alpha\psi$. Since U is unitary, $|\alpha| = 1$ and since U is positivity preserving and ψ is positive, $\alpha = 1$. ∎

For example, if the V_{ij} are all spherically symmetric and H has an eigenvalue at the bottom of its spectrum, that eigenvector is left invariant by rotations and reflections.

We warn the reader that Theorem XIII.46 deals with the lowest eigenvalue of H as an operator on all of $L^2(\mathbb{R}^{3N-3})$. If H commutes with a family $\mathscr{P}$ of permutations of the coordinates and we restrict to a subspace of $L^2(\mathbb{R}^{3N-3})$ with a certain permutation symmetry, then the lowest eigenvalue of the restricted operator need not be nondegenerate. In fact, by the corollary, unless we look at the subspace left *pointwise* invariant by $\mathscr{P}$, the ground state of the restricted operator is an excited state of the unrestricted operator. This implies the statement that *ground states of Boson systems are nondegenerate while ground states of Fermi systems may be degenerate.*

Theorem XIII.47 Let $V \in L^2_{1\infty}(\mathbb{R}^m)$ be positive and suppose $\lim_{|x|\to\infty} V(x) = \infty$. Then $-\Delta + V$ has a nondegenerate strictly positive ground state.

Proof We shall see in Section 14 that $-\Delta + V$ has purely discrete spectrum so the bottom of its spectrum is certainly an eigenvalue. The proof of the remaining conclusions follows closely that of Theorem XIII.46 with one detail different. Let $V_n = \min\{V, n\}$. Then $-\Delta + V_n$, $-\Delta + V$, $-\Delta$, and $-\Delta + (V - V_n)$ are all essentially self-adjoint on $C_0^\infty(\mathbb{R}^m)$ by Theorem X.28. Moreover, for any $\psi \in C_0^\infty(\mathbb{R}^m)$, $V_n\psi \to V\psi$ in L^2. Thus by Theorem VIII.25a we have the necessary strong resolvent convergence. ∎

If V is allowed to be very singular, then $-\Delta + V$, defined as a sum of quadratic forms, can have a degenerate ground state (see Example 2 in Section 13 and Problem 95). A reference for the following result is given in the Notes.

Theorem XIII.48 Let G be a closed subset of $\mathbb{R}^n$ of measure zero and suppose that $V \in L^1_{1\infty}(\mathbb{R}^n\backslash G)$ with $V \geq 0$. Let $H = -\Delta + V$ be defined as the sum of quadratic forms. Then:

(a) If $\mathbb{R}^n\backslash G$ is connected and $\inf \sigma(H)$ is an eigenvalue, then it is a simple eigenvalue and the corresponding eigenfunction is strictly positive.
(b) If $\mathbb{R}^n\backslash G$ is disconnected, V can be chosen so that H has a degenerate ground state.

Finally, we turn to existence and uniqueness of ground states in the framework of hypercontractive semigroups (see Section X.9):

Theorem XIII.49 Let H_0 generate a positivity improving hypercontractive semigroup on a probability measure space $\langle M, \mu \rangle$. Suppose that V is a (not necessarily bounded) multiplication operator with V and e^{-V} in $\bigcap_{p<\infty} L^p(M, d\mu)$. Let $H = H_0 + V$. Then:

(a) $E = \inf \sigma(H)$ is an eigenvalue.
(b) E is nondegenerate.
(c) The ground state eigenfunction is strictly positive.

In particular, (a)–(c) hold for the spatially cutoff $P(\varphi)_2$ Hamiltonians.

Proof We shall first prove (b) and (c) assuming (a) and then prove (a). Let V_n be defined by

$$V_n(q) = \begin{cases} V(q) & \text{if } |V(q)| \leq n \\ n & \text{if } V(q) > n \\ -n & \text{if } V(q) < -n \end{cases}$$

Since $V_n \to V$ in each L^p $(p < \infty)$ and $\sup_n \{\|e^{-V_n}\|_p, \|e^{-(V-V_n)}\|_p\} < \infty$, Theorem X.60 says that $H_0 + V_n \to H_0 + V$ and $H_0 + V - V_n \to H_0$ in norm resolvent sense. Since e^{-tH_0} is a positivity improving semigroup, Theorem XIII.45 is applicable and thus (b) and (c) hold if (a) is true.

To prove (a), we proceed as follows. Let t be chosen so that $A = \exp(-tH)$ is bounded from L^2 to L^4. We need only prove that $\|A\|$ is an eigenvalue of A. A **finite partition** of M is a family $\{S_1, \ldots, S_n\} = \alpha$ of measurable subsets of M that are mutually disjoint, and whose union is M. If α and β are partitions, we write $\beta > \alpha$ if each set in β is a subset of a set in α. For each partition α, define the projection

$$P_\alpha = \sum_{S \in \alpha} \mu(S)^{-1}(\chi_S, \cdot)\chi_S$$

and let $A_\alpha = P_\alpha A P_\alpha$. We first prove the following properties of $\{P_\alpha\}$:

(i) s-$\lim_\alpha P_\alpha = 1$.
(ii) P_α is positivity preserving.
(iii) P_α is a contraction on each $L^p(M, d\mu)$.

To prove (i), we note that for any simple function ψ, $P_\alpha \psi = \psi$ for α sufficiently large. Since the simple functions are dense, (i) follows. (ii) is obvious, and (iii) follows from (ii), $P_\alpha 1 = 1$, and Theorem X.55a. Thus $\{A_\alpha\}$ obeys:

(iv) s-$\lim_\alpha A_\alpha = A$.
(v) $\|A\| = \lim_\alpha \|A_\alpha\|$.
(vi) There is a K with $\|A_\alpha \psi\|_4 \leq K\|A_\alpha\| \, \|\psi\|_2$ for all $\psi \in L^2$ and all α.

(iv) follows from (i). (vi) follows from (iii) and the fact that $\|A\psi\|_4 \leq \tilde{K}\|\psi\|_2$ for some $\tilde{K}$ and the bound $\|A_\alpha\| \geq$ (A1, 1). To prove (v), notice first that $\|A_\alpha\| \leq \|A\|$ since $\|P_\alpha\| = 1$. On the other hand, by (iv), $\|A\| \leq \underline{\lim}\|A_\alpha\|$. Thus $\lim\|A_\alpha\|$ exists and equals $\|A\|$.

Fix a partition $\alpha = \{S_1, \ldots, S_n\}$. Then Ran P_α is naturally isomorphic to $\mathbb{C}^n$ via the map $\sum c_i \chi_{S_i} \mapsto (c_1, \ldots, c_n)$. View $\mathbb{C}^n$ as $L^2(\{1, \ldots, n\}, d\nu)$ with $\nu(i) = \mu(S_i)$. Then A_α is positivity preserving on $\mathbb{C}^n$. Since A_α is a positive definite finite-dimensional matrix, $\|A_\alpha\|$ is an eigenvalue, so we can find $\varphi_\alpha \in$ Ran P_α with $A_\alpha\varphi_\alpha = \|A_\alpha\|\varphi_\alpha$. By the argument in the proof of Theorem XIII.43, $\psi_\alpha = |\varphi_\alpha|$ is an eigenvector. Normalize ψ_α so that $\|\psi_\alpha\|_2 = 1$. Then, on the one hand, $\|\psi_\alpha\|_4 \leq K$, and on the other $1 = \|\psi_\alpha\|_2 \leq \|\psi_\alpha\|_1^{1/3}\|\psi_\alpha\|_4^{2/3}$ by Hölder's inequality. Thus $\|\psi_\alpha\|_1 \geq K^{-2}$. Let ψ be a weak limit point of the net $\{\psi_\alpha\}$, and let $\{\psi_\beta\}$ be a subnet converging to ψ. Then for any $\varphi \in L^2$,

$$(\varphi, A\psi) = (A\varphi, \psi) = \lim_\beta (A\varphi, \psi_\beta) = \lim_\beta \|A_\beta\|(\varphi, \psi_\beta) = \|A\|(\varphi, \psi)$$

so $A\psi = \|A\|\psi$. Moreover, since $\psi_\beta \geq 0$, $\|\psi_\alpha\|_1 = (1, \psi_\alpha) \geq K^{-2}$. Thus $(1, \psi) \geq K^{-2}$. In particular, $\psi \neq 0$. Thus $\|A\|$ is an eigenvalue. ∎

Appendix 1 to Section XIII.12 The Beurling-Deny criteria

There is an especially simple criterion for a positive self-adjoint operator H on $L^2(M, d\mu)$ to generate a positivity preserving semigroup.

Theorem XIII.50 (first Beurling–Deny criterion) Let $H \geq 0$ be a self-adjoint operator on $L^2(M, d\mu)$. Extend $(\psi, H\psi)$ to all of L^2 by setting it equal to infinity when $\psi \notin Q(H)$. Then the following are equivalent:

(a) e^{-tH} is positivity preserving for all $t > 0$.
(b) $(|u|, H|u|) \leq (u, Hu)$ for all $u \in L^2$.
(c) e^{-tH} is reality preserving and

$$(u_+, Hu_+) \leq (u, Hu)$$

for all real-valued $u \in L^2$. Here $u_+(x) \equiv \max\{u(x), 0\}$.
(d) e^{-tH} is reality preserving and

$$(u_+, Hu_+) + (u_-, Hu_-) \leq (u, Hu)$$

for all real-valued $u \in L^2$. Here $u_- = u_+ - u$.

Proof We shall prove that (a) ⇒ (b) ⇒ (a). The proofs that (a) ⇒ (d) and (c) ⇒ (a) are similar and left to the reader (Problem 96).

(a) ⇒ (b) With our convention on extending $(\cdot, H\cdot)$ to L^2,

$$(u, Hu) = \lim_{t \to 0} t^{-1}[(u, (1 - e^{-tH})u)] \tag{73}$$

By hypothesis (a), $|e^{-tH}u| \leq e^{-tH}|u|$, so

$$(u, e^{-tH}u) = \|e^{-tH/2}u\|^2 \leq \|e^{-tH/2}|u|\|^2 = (|u|, e^{-tH}|u|)$$

Thus, since $(u, u) = (|u|, |u|)$, we have that

$$(u, (e^{-tH} - 1)u) \leq (|u|, (e^{-tH} - 1)|u|)$$

so that (b) follows from (73).

(b) ⇒ (a) Suppose that u is a positive function and that $a > 0$. Let $w = (H + a)^{-1}u$ and define $Q(\varphi) = (\varphi, H\varphi) + a(\varphi, \varphi)$ on all of L^2. One first notes that for $\varphi \in D(H)$ and any ψ,

$$Q(\varphi + \psi) = Q(\varphi) + Q(\psi) + 2\,\mathrm{Re}((H + a)\varphi, \psi)$$

Thus, if $\mathrm{Re}\, v \geq 0$,

$$Q(w + v) = Q(w) + Q(v) + 2\,\mathrm{Re}(u, v) \geq Q(w) + Q(v)$$

Put differently, if $\varphi \equiv w + v$ obeys $\mathrm{Re}\,\varphi \geq \mathrm{Re}\, w$, then $Q(\varphi) \geq Q(w)$ with equality only if $\varphi = w$. By hypothesis (b), $Q(|w|) \leq Q(w)$. Since $\mathrm{Re}\,|w| \geq \mathrm{Re}\, w$, we see that $|w| = w$, that is, $w \geq 0$. We have thus seen that $(H + a)^{-1}$ is positivity preserving for any $a > 0$. Therefore, by the proposition preceding Theorem XIII.44, the semigroup is positivity preserving. ∎

Example 1 Criterion (d) implies that a finite-dimensional positive definite matrix generates a positivity preserving semigroup if and only if its off-diagonal elements are all negative. This is quite easy to prove directly in a more general form (Problem 97).

Example 2 One can see directly, without appealing to the Trotter product formula, that if V is a positive multiplication operator and H_0 generates a positivity preserving semigroup, then so does $H_0 + V$ defined as a sum of forms. For, when $Q(H) = Q(H_0)$, criterion (b) holds for H_0 if and only if it holds for H.

Example 3 It is easy to see (Problem 99) that the Dirichtlet and Neumann Laplacians defined in Section 15 obey criterion (b) and thus generate positivity preserving semigroups; equivalently, the integral kernels of their resolvents ("Green's functions") are positive functions.

There is a slightly more subtle criterion for e^{-tH} to be a contraction on all the L^p spaces as well as positivity preserving.

Theorem XIII.51 (second Beurling–Deny criterion) Let $H \geq 0$ be a self-adjoint operator that generates a positivity preserving semigroup on $L^2(M, d\mu)$. Then the following are equivalent:

(a) e^{-tH} is a contraction on each $L^p(M, d\mu)$ for all p and all $t \geq 0$.
(b) e^{-tH} is a contraction on $L^\infty(M, d\mu)$ for all $t > 0$.
(c) Let $(f \wedge 1)(x) \equiv \min\{f(x), 1\}$. For each $f \geq 0$,

$$((f \wedge 1), H(f \wedge 1)) \leq (f, Hf)$$

(d) Let F be an arbitrary function from $\mathbb{C}$ to $\mathbb{C}$ obeying $|F(x)| \leq |x|$ and $|F(x) - F(y)| \leq |x - y|$. Then

$$(F(f), HF(f)) \leq (f, Hf)$$

for all $f \in L^2$.

Proof We shall show that (c) $\Rightarrow$ (b) and (a) $\Rightarrow$ (d). The implication (b) $\Rightarrow$ (a) follows by a simple modification of the duality interpolation argument used in the proof of Theorem X.55a, and (d) $\Rightarrow$ (c) follows if we note that $F(z) = \min\{\text{Re } z, 1\}$ obeys the restrictions on F.

(c) $\Rightarrow$ (b) Fix $u \in L^2$ with $0 \leq u \leq 1$. Define

$$\psi(v) = (v, Hv) + \|u - v\|^2 = (v, (H + 1)v) + \|u\|^2 - 2 \text{ Re}(u, v)$$

Let $R = (H + 1)^{-1}$. Then $\psi(Ru) = \|u\|^2 - (u, Ru)$ and

$$((Ru - v), (H + 1)(Ru - v)) = (u, Ru) + (v, (H + 1)v) - 2 \text{ Re}(u, v)$$

so we have

$$\psi(v) = \psi(Ru) + ((Ru - v), (H + 1)(Ru - v))$$

This says that $\psi(v)$ takes its minimum value when and only when $v = Ru$. Now, since $u \leq 1$,

$$|(u - (v \wedge 1))(x)| \leq |(u - v)(x)|$$

and, by hypothesis $(v \wedge 1, H(v \wedge 1)) \leq (v, Hv)$ if $v \geq 0$. Thus

$$\psi(Ru \wedge 1) \leq \psi(Ru)$$

Since Ru minimizes ψ, we have that $Ru \wedge 1 = Ru$, i.e., $Ru \leq 1$. Thus R is a contraction on L^∞. Similarly, $(1 + \varepsilon H)^{-1}$ is a contraction on L^∞ for all ε so that $e^{-tH} = \lim(1 + tH/n)^{-n}$ is a contraction on L^∞.

$(a) \Rightarrow (d)$ By (73), it clearly suffices to show that

$$(F(f), (1 - e^{-tH})F(f)) \leq (f, (1 - e^{-tH})f)$$

for all $t > 0$. Let K be a finite-dimensional subspace of $L^2(M, d\mu)$ of functions of the form $\sum_{i=1}^n \alpha_i \chi_{A_i}$ where $\{A_i\}_{i=1}^n$ are disjoint sets of finite measure. Under the order $K' > K$ if $K \subset K'$, the set of such K's is a directed set. If $P(K)$ is the projection onto K, s-$\lim_K P(K) = 1$, so it suffices to prove that

$$(F(P(K)f), (1 - e^{-tH})F(P(K)f)) \leq (P(K)f, (1 - e^{-tH})P(K)f)$$

for each K. Let

$$b_{ij} = (\chi_{A_i}, (1 - e^{-tH})\chi_{A_j})$$

Then we need only prove that

$$\sum_{i,j} \overline{F(\alpha_i)} F(\alpha_j) b_{ij} \leq \sum_{i,j} \bar{\alpha}_i \alpha_j b_{ij} \tag{74}$$

Let $\lambda_i = (\chi_{A_i}, \chi_{A_i})$ and $a_{ij} = (\chi_{A_i}, e^{-tH}\chi_{A_j})$. Then $a_{ij} \geq 0$ and since $\|e^{-tH}\chi_{A_j}\|_1 \leq \lambda_j$, we have

$$\sum_i a_{ij} \leq \lambda_j$$

Let $m_j = \lambda_j - \sum_i a_{ij} \geq 0$. Then $b_{ij} = \lambda_i \delta_{ij} - a_{ij}$, so

$$\sum_{i,j} \bar{z}_i z_j b_{ij} = \sum_{i<j} a_{ij} |z_i - z_j|^2 + \sum_j m_j |z_j|^2$$

From this representation, (74) follows. ∎

Example 3, revisited Using criterion (c), it is easily seen that Neumann and Dirichlet Laplacians generate contraction semigroups on L^p (Problem 99).

Appendix 2 to XIII.12 The Levy–Khintchine formula

In order to apply the theorems of Section 12 one needs methods of proving that semigroups are positivity preserving. If the generator is of the form $-\Delta + V(x)$, then, as we have seen, the generated semigroup is positivity

preserving since the explicit representation of $e^{t\Delta}$ on $L^2(\mathbb{R}^n)$ shows that it is positivity preserving and the Trotter product formula allows us to conclude from this that $e^{t(\Delta - V)}$ is positivity preserving also. It is a natural question to ask for what other functions $F(-i\nabla)$ the operator $F(-i\nabla) + V(x)$ generates a positivity preserving semigroup. Certainly, if

$$F(-i\nabla) = -\sum_{i,j=1}^{n} a_{ij} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} + c$$

where $\{a_{ij}\}$ is a strictly positive definite matrix, the answer is yes since by change of variables $F(-i\nabla)$ can be reduced to $-\Delta + c$. However, it is not clear a priori which other functions F are allowed.

Let F be a continuous complex-valued function on $\mathbb{R}^n$ whose real part is bounded from below. As in Section IX.7, we define

$$F(-i\nabla)\varphi = \widetilde{F(p)\hat{\varphi}}$$

Because of the semiboundedness of the real part of F, $F(-i\nabla)$ generates a strongly continuous semigroup on $L^2(\mathbb{R}^n)$. For V's that are not too nasty, Theorem X.50 shows that $F(-i\nabla) + V(x)$ also generates a strongly continuous semigroup and the Trotter product formula (Theorem X.51) reduces the question of whether $\exp(-t(F(-i\nabla) + V(x)))$ is positivity perserving to the same question for $\exp(-tF(-i\nabla))$. The point of this appendix is to characterize in different ways the set of F's so that this is true.

First, set $G(x) = e^{-tF(x)}$ and let f and g be positive functions in $\mathscr{S}(\mathbb{R}^n)$. Then,

$$\begin{aligned}(f, G(-i\nabla)g) &= (\widetilde{G(p)\hat{g}})(f) \\ &= (2\pi)^{-n/2}(\check{G} * g)(f) \\ &= (2\pi)^{-n/2}(\check{G} * (g * \tilde{f}))(0)\end{aligned}$$

Thus, if $\check{G}$ is a polynomially bounded positive measure, then $(f, G(-i\nabla)g) \geq 0$ for such f and g. Thus, by the Bochner–Schwartz theorem (Theorem IX.10), if G is positive definite, then $G(-i\nabla)$ is positivity preserving. Conversely, if $G(-i\nabla)$ is positivity preserving and we set $g_y(x) = f(x + y)$, then

$$\begin{aligned}(2\pi)^{-n/2}(\check{G} * f * \tilde{f})(y) &= (2\pi)^{-n/2}(\check{G} * g_y * \tilde{f})(0) \\ &= (f, G(-i\nabla)g_y) \\ &\geq 0\end{aligned}$$

Since $\check{G}$ is tempered, the left-hand side is a polynomially bounded function (Theorem IX.4a). Thus by Bochner's theorem, $\mathscr{F}(\check{G} * f * \tilde{f}) = (2\pi)^n |\hat{f}|^2 G$ is a positive definite function. If we now let $f(x) = j_\varepsilon(x)$, an approximate identity, then as $\varepsilon \downarrow 0$, $|\hat{j}_\varepsilon|^2 G \to G$ uniformly on compact sets, so G is positive definite.

This proves the first of the characterizations given by the following theorem. The second equivalence gives a characterization in terms of F itself.

Theorem XIII.52 Let $F(x)$ be a complex-valued function on $\mathbb{R}^n$ whose real part is bounded below. Then the following are equivalent:

(a) $e^{-tF(-i\nabla)}$ is a positivity preserving semigroup.
(b) For each $t > 0$, $e^{-tF(x)}$ is a positive definite distribution in the sense of Bochner.
(c) $\overline{F(x)} = F(-x)$ and

$$\sum_{i,j=1}^{m} F(\mathbf{x}_i - \mathbf{x}_j)\bar{z}_i z_j \leq 0 \tag{75}$$

for all $\mathbf{x}_1, \ldots, \mathbf{x}_m \in \mathbb{R}^n$ and $\mathbf{z} \in \mathbb{C}^m$ satisfying $\sum_{i=1}^m z_i = 0$.

Proof We have already proven that (a) and (b) are equivalent. In order to prove that (b) and (c) are equivalent it is sufficient to show that if $A = \{a_{ij}\}$ is an $m \times m$ matrix and $M(t)$ is the matrix with entries $M(t)_{ij} = e^{ta_{ij}}$, then $M(t)$ is positive definite for all $t \geq 0$ if and only if A is **conditionally positive definite**, i.e., $(A\zeta, \zeta) \geq 0$ for all $\zeta \in \mathbb{C}^m$ satisfying $\sum_{i=1}^m \zeta_i = 0$. So, suppose that $M(t)$ is positive definite for $t \geq 0$ and let $\sum_{i=1}^m \zeta_i = 0$. Then $(\zeta, M(t)\zeta) = 0$ at $t = 0$ and $(\zeta, M(t)\zeta) \geq 0$ for $t \geq 0$. Therefore,

$$(\zeta, A\zeta) = \frac{d}{dt}(\zeta, M(t)\zeta)\Big|_{t=0} \geq 0$$

so A is conditionally positive definite.

Conversely, suppose that A is conditionally positive definite. Let e be the vector whose components all equal $1/\sqrt{m}$ and let P be the projection onto the orthogonal complement of e. The hypothesis on A is that PAP is positive definite. Thus, if we define $\tilde{a}_{ij} = (PAP)_{ij}$ and write

$$A = PAP + (1 - P)A(1 - P) + PA(1 - P) + (1 - P)AP$$

then one can easily check that

$$a_{ij} = \tilde{a}_{ij} + \bar{b}_i + b_j$$

for some vector b. Therefore, $M(t)_{ij} = \tilde{M}(t)_{ij} C(t)_{ij}$ where $\tilde{M}(t)_{ij} = e^{t\tilde{a}_{ij}}$ and $C(t)_{ij} = e^{t\bar{b}_i} e^{tb_j}$. Now, using the lemma below inductively, we have that $\{e^{D_{ij}}\}$

is positive definite if $\{D_{ij}\}$ is positive definite. Applying this result we see that $\tilde{M}(t)_{ij}$ is positive definite. $C(t)_{ij}$ is obviously positive definite, so using the lemma again we conclude that $\{M(t)_{ij}\}$ is positive definite. ∎

The proof of the theorem is completed by the following lemma.

Lemma Let $\{D_{ij}\}$ and $\{F_{ij}\}$ be positive definite matrices. Then $\{D_{ij}F_{ij}\}$ is positive definite.

Proof Let $\{\mu_k, d_k\}$ and $\{\lambda_\ell, f_\ell\}$ be the eigenvalues and corresponding eigenfunctions of $\{D_{ij}\}$ and $\{F_{ij}\}$ respectively. If $\{e_i\}$ is the standard basis in $\mathbb{C}^n$, then

$$D_{ij}F_{ij} = \sum_{\ell,k=1}^{n} \mu_k \lambda_\ell (e_i, d_k)(e_i, f_\ell)(d_k, e_j)(f_\ell, e_j)$$

Now, fix k and ℓ and let $s_i = (e_i, d_k)(e_i, f_\ell)$. Then $\{s_i \bar{s}_j\}$ is positive definite. Therefore, $\{D_{ij}F_{ij}\}$ is positive definite since it a sum (with positive coefficients) of positive definite matrices. ∎

Functions that satisfy (75) are called **conditionally negative definite**. Although we have characterized the functions in which we are interested, it is very important to have other characterizations since, first, (75) is not easy to check, and secondly, it is hard to extract other necessary conditions from (75). Two further characterizations are given by the following theorem.

Theorem XIII.53 Let $F(x)$ be a complex-valued function on $\mathbb{R}^n$ whose real part is bounded below. Then the following are equivalent:

(a) $e^{-tF(-i\nabla)}$ is a positivity preserving semigroup.

(b) For each $a \in \mathbb{C}^n$, $-D^*DF$ is a positive definite distribution, where $D = \sum_{i=1}^n a_i \partial_i$ and $D^* = -\sum_{i=1}^n \bar{a}_i \partial_i$.

(c) (the Levy–Khintchine formula) There exists a positive finite measure ν on $\mathbb{R}^n$, with $\nu(\{0\}) = 0$, a positive definite matrix $A = \{a_{ij}\}$, a real vector $\boldsymbol{\beta}$, and a real number α so that

$$F(\mathbf{x}) = \alpha + i\boldsymbol{\beta} \cdot \mathbf{x} + \mathbf{x} \cdot A\mathbf{x} - \int_{\mathbb{R}^n} \left[e^{i\mathbf{x}\cdot\mathbf{y}} - 1 - \frac{i\mathbf{x}\cdot\mathbf{y}}{1+y^2} \right] \frac{1+y^2}{y^2} d\nu(\mathbf{y}) \quad (76)$$

Proof We shall show that (75) is equivalent to (b) and to (c). So, suppose that (75) holds. Then a simple approximation argument shows that

$$F(\quad * f) = \int F(x-y) f(x) \overline{f(y)}\, dx\, dy \leq 0$$

for any $f \in C_0^\infty(\mathbb{R}^n)$ that satisfies $\int f(x)\,dx = 0$. Now, if $D = \sum a_i\,\partial_i$, then $\int Df(x)\,dx = 0$ for all $f \in C_0^\infty(\mathbb{R}^n)$, so

$$0 \leq -F(\widetilde{Df} * Df) = -F(D^*D(\tilde{f} * f)) = -D^*DF(\tilde{f} * f)$$

Thus, $-D^*DF$ is a positive definite distribution.

We now show that (b) implies (c). Although the idea is simple, this is the lengthiest part of the proof. First, there are some complications with the multidimensional case; and secondly, there are technical complications caused by the fact that a priori F is only an ordinary distribution. Since we want to deal with the Fourier transform of F, we introduce the space $\mathscr{Z}$ of Fourier transforms of functions in C_0^∞ with the topology $g_\alpha \to g$ in $\mathscr{Z}$ if and only if $\check{g}_\alpha \to \check{g}$ in C_0^∞. $\mathscr{Z}$ has an intrinsic description on account of the Paley–Wiener theorem (Theorem IX.11), but that will not concern us. Let G, "the Fourier transform of F," be defined as the linear functional on $\mathscr{Z}$ given by

$$(G, g) = (F, \hat{g})$$

Choose a function $\alpha \in \mathscr{Z}$ so that $\alpha(x) = 1 + O(x^3)$ at $x = 0$. To see that such an α exists, first choose any $\beta \in \mathscr{Z}$ with $\beta(0) = 1$. Then

$$\beta(x) = 1 + \sum_i b_i x_i + \sum_{i,j} a_{ij} x_i x_j + O(x^3)$$

Let $p(x)$ be the polynomial $p(x) = 1 + \sum c_i x_i + \sum_{i,j} d_{ij} x_i x_j$ with $c_i = -b_i$; $d_{ij} = -a_{ij} + b_i b_j$. Then $\alpha(x) = p(x)\beta(x)$ lies in $\mathscr{Z}$ since C_0^∞ is closed under the application of differential operators, and $\alpha(x) = 1 + O(x^3)$.

Our goal will be to prove that there is a tempered positive measure σ and real numbers a_0, b_i $(i = 1, \ldots, n)$, $c_{ij} (i, j = 1, \ldots, n)$ so that

$$(2\pi)^{n/2} F(x) = -\int_{|\lambda|>0} [e^{i\lambda \cdot x} - \alpha(\lambda)(1 + i\lambda \cdot x)]\,d\sigma(\lambda) + a_0 + i\sum_{j=1}^n b_j x_j + \sum_{i,j=1}^n c_{ij} x_i x_j \tag{77}$$

with $\{c_{ij}\}$ a positive definite matrix and

$$\int_{0<|\lambda|\leq 1} |\lambda|^2\,d\sigma + \int_{|\lambda|\geq 1} d\sigma < \infty$$

We leave the rewriting of (77) into the form (76) to the reader (Problem 100).

Letting G be the Fourier transform of F, (77) is clearly equivalent to

$$(G, \varphi) = -\int_{|\lambda|>0} [\varphi(\lambda) - \alpha(\lambda)(\varphi(0) + \lambda \cdot \nabla\varphi(0))]\, d\sigma(\lambda)$$

$$+ a_0 \varphi(0) + \sum_{j=1}^{n} b_j(\partial_j\varphi)(0) - \sum_{i,\, j=1}^{n} c_{ij}(\partial_i\, \partial_j\varphi)(0) \qquad (78)$$

for all $\varphi \in \mathscr{X}$. Suppose that we can prove that

$$(G, \varphi) = -\int_{|\lambda|\geq 0} \varphi(\lambda)\, d\sigma(\lambda) - \sum_{i,\, j=1}^{n} c_{ij}(\partial_i\, \partial_j\varphi)(0) \qquad (79)$$

for all φ that vanish to order one at $\lambda = 0$. Then (78) follows by applying (79) to $\varphi(\lambda) - \alpha(\lambda)[\varphi(0) + \lambda \cdot \nabla\varphi(0)]$. Next we note that the right-hand side of (79) defines a continuous functional on $\{\varphi \in \mathscr{X} \,|\, \varphi(0) = 0 = \partial_j\varphi(0),\ j = 1, \ldots, n\}$ as long as

$$\int_{0<|\lambda|\leq 1} |\lambda|^2\, d\sigma + \int_{|\lambda|\geq 1} d\sigma < \infty$$

(Problem 101) and that the sums of functions of the form $\lambda_i\lambda_j\psi$ with $\psi \in \mathscr{X}$ are the same as those $\varphi \in \mathscr{X}$ satisfying $\varphi(0) = 0 = \partial_j\varphi(0)$ (Problem 102).

Thus, to prove (76) it suffices to prove that there is a measure $d\sigma$ with the required bound, and a positive definite matrix c_{ij} so that (79) holds for all φ of the form $\lambda_i\lambda_j\psi$ with $\psi \in \mathscr{X}$. We first claim that there is a signed measure dv_{ij} on $\mathbb{R}^n$ so that

$$(G, \lambda_i\lambda_j\psi) = -\int \psi(\lambda)\, dv_{ij}(\lambda) \qquad (80)$$

for all $\psi \in \mathscr{X}$. For $-(\lambda_i \pm \lambda_j)^2 G$ defines a tempered positive measure by hypothesis (b), Bochner's theorem, and

$$\lambda_i\lambda_j = \tfrac{1}{4}[(\lambda_i + \lambda_j)^2 - (\lambda_i - \lambda_j)^2]$$

Since

$$(G, \lambda_i\lambda_j(\lambda_k\lambda_\ell\eta)) = (G, \lambda_k\lambda_\ell(\lambda_i\lambda_j\eta))$$

we see that the measures dv_{ij} obey the condition

$$\lambda_k\lambda_\ell\, dv_{ij} = \lambda_i\lambda_j\, dv_{k\ell} \qquad (81)$$

We can therefore define a measure $d\sigma$ on $\mathbb{R}^n\backslash\{0\}$ which is tempered at ∞ so that $\int_{0<|\lambda|<1} |\lambda|^2\, d|\sigma| < \infty$ as follows: Let $\Omega_{ij} = \{\lambda \,|\, \lambda_i\lambda_j \neq 0\}$. On Ω_{ij}, let

$d\mu = (\lambda_i \lambda_j)^{-1}\, dv_{ij}$. By (81) this measure is a well-defined measure on $\bigcup \Omega_{ij} = \mathbb{R}^n \backslash \{0\}$. In particular, by (81), $\mu\{\lambda \mid \lambda_i \lambda_j = 0;\ \lambda \neq 0\} = 0$, so by (80),

$$(G, \lambda_i \lambda_j \psi) = -\int_{|\lambda|>0} (\lambda_i \lambda_j \psi(\lambda))\, d\mu - v_{ij}(\{0\})\psi(0)$$

Now, setting $\varphi = \lambda_i \lambda_j \psi$, $\psi(0) = (\partial_i\, \partial_j \varphi)(0)$ and moreover, $(\partial_k\, \partial_\ell \varphi)(0) = 0$ unless $\{k, \ell\} = \{i, j\}$. Thus, (79) is proven with $c_{ij} = v_{ij}(\{0\})$.

All that remains is to prove that $d\sigma$ is positive with $\int_{|\lambda|>1} d\sigma < \infty$ and that $\{c_{ij}\}$ is positive definite. To see that σ is positive, we note that by hypothesis, $\lambda_i^2\, d\sigma$ is positive for each i and so $\lambda^2\, d\sigma$ is positive. Moreover, for any $\zeta \in \mathbb{C}^n$, $\sum \bar{\zeta}_i \zeta_j c_{ij} = v_\zeta(\{0\}) \geq 0$ where v_ζ is the Fourier transform of $-D_\zeta^* D_\zeta F$ with $D_\zeta = \sum_{i=1}^n \zeta_i\, \partial_i$. Finally, $\int_{|\lambda|>1} d\sigma < \infty$ by an argument (Problem 103) based on the formal relation $F(0) = -\int_{|\lambda|>0} (1 - \alpha(\lambda))\, d\sigma + a_0$. We have therefore proven that (b) implies (c).

It remains to show that the Levy–Khintchine formula implies (75). First, we claim that

$$\left| e^{ixy} - 1 - \frac{ixy}{1+y^2} \right| \leq C\left[\frac{y^2}{1+y^2}\right](1+x^2) \tag{82}$$

For, when $|y| \geq 1$, the left-hand side is bounded by $2 + \frac{1}{2}x$ and when $|y| \leq 1$ by $C|xy|^2 + |xy|(y^2/(1+y^2))$. From (82) any F of the form (76) is a tempered distribution satisfying

$$|F(x)| \leq C(1 + |x|^2) \tag{83}$$

and by a direct calculation each distribution $-(D^*D)F$ is positive definite. Since F is tempered, it has a Fourier transform $\hat{F}$. Moreover, as in the proof that (b) implies (c), the Fourier transform of $\partial_i\, \partial_j F$ is a signed measure dv_{ij} with $dv_\zeta = \sum \bar{\zeta}_i \zeta_j\, dv_{ij}$ a positive measure for each $\zeta \in \mathbb{C}^n$. Thus, for any functions $f_i(k)$ $(i = 1, .\,, n)$,

$$\sum_{i,j} \int \overline{f_i(k)} f_j(k)\, dv_{ij}(k) \geq 0$$

Now suppose that $\int f(x)\, dx = 0$. Then $\hat{f}(0) = 0$ so, by a simple argument, $\hat{f}(k) = \sum k_i\, f_i(k)$ with $f_i(k) \in \mathcal{S}$. It follows that

$$\int F(x-y)\overline{f(x)} f(y)\, dx\, dy = -\sum_{i,j} \int \overline{f_i(k)} f_j(k)\, dv_{ij}(k) \leq 0 \quad \blacksquare$$

Example 1 We now answer the question of which self-adjoint constant coefficient partial differential operators generate positivity preserving semigroups. Let $F(p)$ be a polynomial in n variables that is bounded below, and

suppose that $\exp(-tF(-i\mathbf{V}))$ is positivity preserving. Then by Theorem XIII.52, F is conditionally negative definite and by (83), F must have order less than or equal to two. Furthermore, the self-adjointness condition $\overline{F(p)} = F(p)$ and the condition $F(p) = F(-p)$ (from (75)) imply that the first-order terms are absent. Thus, $F(p) = \sum a_{ij} p_i p_j + c$. Finally, for $\zeta \in \mathbb{C}^n$ and $D_\zeta = \sum_{i=1}^n \zeta_i \partial_i$, we have

$$(D_\zeta^* D_\zeta F)(0) = -\sum a_{ij} \zeta_i \zeta_j$$

Since $D_\zeta^* D_\zeta F$ is negative definite by part (b) of Theorem XIII.53, $\{a_{ij}\}$ must be positive definite. Thus, the *only* constant coefficient self-adjoint partial differential operators that generate positivity preserving semigroups are of the form

$$F(-i\mathbf{V}) = -\sum_{i=1}^{n} a_{ij} \partial_i \partial_j + c$$

where $\{a_{ij}\}$ is positive definite. On the other hand, each of these may be reduced by change of variables to $-\Delta + c$ so they all do generate positivity preserving semigroups.

From this example it is clear that if we want to find new conditionally negative functions (that satisfy $\overline{F(p)} = F(p)$) we have to look further than polynomials. To do this, it is useful to simplify condition (b) of Theorem XIII.53.

Theorem XIII.54 Suppose that F is a spherically symmetric, polynomially bounded continuous function satisfying $F(0) = 0$. Suppose further that ΔF is positive definite. Then F is conditionally negative definite.

Proof Let $G = -\hat{F}$. Thus $k^2 G$ is a polynomially bounded positive measure. So G extends from $\mathcal{S}(\mathbb{R}^n)$ to a set including all functions of the form $k^2 f(k)$ where f is continuous and $k^n f(k) \to 0$ as $|k| \to \infty$. In particular, if $g \in \mathcal{S}$, then

$$k_i k_j k_\ell g = k^2[(k_i k_j k_\ell)k^{-2}]g$$

has this form and thus as in the proof of Theorem XIII.53, there is a measure μ on $\mathbb{R}^n \backslash \{0\}$ so that

$$G(k_i k_j k_\ell g) = \int k_i k_j k_\ell g(k)\, d\mu$$

for all g in $\mathscr{S}$. Moreover, $\int_{|k|\le 1} k^2\, d\mu(k) < \infty$. Thus, as in the proof of Theorem XIII.53,

$$G(f) = \int_{|\lambda|>0} [\varphi(\lambda) - \alpha(\lambda)(\varphi(0) + \lambda \cdot \nabla\varphi(0) + \tfrac{1}{2}\sum \lambda_i\lambda_j\, \partial_i\partial_j\varphi(0))]\, d\mu$$

$$- a_0\varphi(0) - \sum_{j=1}^{n} b_j\, \partial_j\varphi(0) + \sum_{i,\,j=1}^{n} c_{ij}(\partial_i\, \partial_j\varphi)(0)$$

where $\alpha \in C_0^\infty$ is identically 1 near 0. Since $\int k^2\, d\mu(k) < \infty$, we can eliminate the $\lambda_i\lambda_j(\partial_i\, \partial_j\varphi)(0)$ term in the integral and absorb it into the c_{ij} term. Thus

$$(2\pi)^{n/2}F(x) = -\int_{|\lambda|>0} [e^{i\lambda x} - \alpha(\lambda)(1 + \lambda \cdot x)]\, d\mu(\lambda) \tag{84}$$

$$+ \alpha_0 + i\beta \cdot x + \sum_{i,\,j} \gamma_{ij}x_i x_j$$

so to prove that F is conditionally negative definite, we need only prove that γ_{ij} is positive definite. Since F is rotationally invariant and α can be chosen rotationally invariant, γ_{ij} must equal $\gamma\delta_{ij}$ so we need only prove that $\gamma > 0$. But the Fourier transform of ΔF is $d\nu = \lambda^2\, d\mu + 2\delta(\lambda)\mathrm{Tr}(\gamma_{ij})$ so $n\gamma = \mathrm{Tr}(\gamma_{ij}) = \frac{1}{2}\nu(\{0\})$ is positive. ∎

Example 2 We claim that

$$F_1(p) = |p|^\alpha; \qquad 1 \le \alpha \le 2 \quad \text{if } n = 1, \qquad 0 \le \alpha \le 2 \quad \text{if } n > 1$$

$$F_2(p) = \sqrt{p^2 + m^2}; \qquad m > 0$$

are conditionally positive definite. For we can compute ΔF in both cases and find:

$$\Delta F_1(p) = \alpha(n + \alpha - 2)|p|^{\alpha-2}$$

$$\Delta F_2(p) = (n-1)(p^2 + m^2)^{-1/2} + m^2(p^2 + m^2)^{-3/2}$$

So we need only prove that $|p|^{\alpha-2}$, $(p^2 + m^2)^{-1/2}$ and $(p^2 + m^2)^{-3/2}$ are positive definite. Now, p^2 is conditionally positive definite, so e^{-tp^2} is positive definite. Since, for $\alpha < 2$,

$$|p|^{\alpha-2} = c_\alpha \int_0^\infty t^{-\alpha/2}e^{-tp^2}\, dt$$

$|p|^{\alpha-2}$ is positive definite as the integral of positive definite functions convergent as an integral of distributions. Similarly, for $\beta > 0$,

$$(p^2 + m^2)^{-\beta} = d_\beta \int_0^\infty t^{\beta-1}e^{-t(p^2+m^2)}\, dt$$

so $(p^2 + m^2)^{-\beta}$ is positive definite for $\beta > 0$.

The choice for the free Hamiltonian $h_0 = (p^2 + m^2)^{1/2} - m$ is of some interest since it is the quantum analogue of the energy of a relativistic particle. It should describe spinless particles (e.g., pions) in the region where relativity is of some importance but where particle creation phenomena (field theoretic effects) are not yet important.

Our last topic is an aside from the main motivation of this appendix, but we include it because of its importance to probability theory.

Definition A probability measure μ on $\mathbb{R}^n$ is called **infinitely divisible** if for any n, there is a probability measure ν_n with $\mu = \nu_n * \nu_n * \cdots * \nu_n$ (n times). The Fourier transforms of probability measures are called **characteristic functions**. A characteristic function $f(x)$ is called **infinitely divisible** if for each n, there is a characteristic function $f_n(x)$ so that $f(x) = (f_n(x))^n$.

What we would like to do is to characterize those functions that are infinitely divisible characteristic functions. Let F be continuous. First, notice that if $e^{-tF(p)}$ is positive definite for all $t > 0$, then $e^{-F(p)}$ is an infinitely divisible characteristic function. But the converse is also true. For suppose that $e^{-F(p)}$ is infinitely divisible. Then, there is a positive definite function g_2 so that $g_2(p)^2 = e^{-F(p)}$. Clearly, $g_2(p) = \pm\exp(-\frac{1}{2}F(p))$ for all p. Since g_2 and F are continuous and $g_2(0) = 1 = +\exp(-\frac{1}{2}F(0))$, the plus sign always occurs. In this way we see that $\exp(-2^{-n}F)$ is positive definite for all n. Since products and limits of positive definite functions are positive definite, we conclude that $\exp(-tF(p))$ is positive definite for all t. This remark combined with the theorems that we have already proven allow us to characterize infinitely divisible characteristic functions.

Theorem XIII.55 (the Levy–Khintchine theorem) Every infinitely divisible characteristic function G is of the form $G = e^{-F}$ for some F satisfying (76).

Proof Let G_m be the positive definite function with $(G_m)^m = G$. Then $G_m(0) = 1$ and since G is continuous, $G(x) \neq 0$ for $|x| < \varepsilon$ for suitable ε. Thus $G_m(x) \to 1$ for $|x| < \varepsilon$ as $m \to \infty$. By the lemma below, $G_m(x) \to 1$ for *all* x so that G is never zero. By a fundamental topological property of $\mathbb{R}^n$, any nonvanishing complex-valued continuous function on $\mathbb{R}^n$ has a unique continuous logarithm once it is fixed at one point. Thus, there is a unique continuous function F with $G = e^{-F}$ and $F(0) = 0$. Since G is bounded, the real part of F is bounded below. By the remark before the theorem, $\exp(-tF(x))$ is positive definite for all $t > 0$, so by Theorem XIII.52, $e^{-tF(-i\nabla)}$ is a positivity preserving semigroup. Thus, by Theorem XIII.53, there is a finite positive measure so that the Levy–Khintchine formula (76) holds. ∎

Lemma Let G_m be a sequence of positive definite fuctions with $G_m(0) = 1$. Suppose that as $m \to \infty$, $G_m(x) \to 1$ for x in some neighborhood of zero. Then $G_m(x) \to 1$ for all x.

Proof By hypothesis, there exist measures μ_m on $\mathbb{R}^n$ with

$$G_m(x) = \int e^{ixy}\, d\mu_m(y)$$

By hypothesis, each μ_m has mass 1. Moreover, an elementary use of Fubini's theorem shows that

$$(2a)^{-n} \int_{|x_i| \le a} [1 - G_m(x)]\, dx = \int \left(1 - \prod_{i=1}^{n} \frac{\sin\, ay_i}{ay_i}\right) d\mu_m(y)$$

$$\geq C\mu_m\{y \,|\, y_i \geq a^{-1} \text{ for some } i\}$$

where $C = \min_{y \geq 1} (1 - y^{-1} \sin\, y) > 0$. Thus, by the hypothesis on G_m, for some a, $\mu_m\{y \,|\, y_i \geq a^{-1}$ for some $i\} \to 0$ as $m \to \infty$. View the μ_m as measures on $\dot{\mathbb{R}}^n$, the one-point compactification of $\mathbb{R}^n$. Let μ_∞ be any weak limit point of the μ_m; such limit points exist since $\mathscr{M}_{+,1}(\dot{\mathbb{R}}^n)$ is compact. Since $\mu_m\{y \,|\, |y| \geq a^{-1}\} \to 0$ as $m \to \infty$ for some a, we can conclude that μ_∞ is a measure on $\mathbb{R}^n$, i.e., $\mu_\infty(\{\infty\}) = 0$ and that $\int f(y)\, d\mu_{m(i)} \to \int f(y)\, d\mu_\infty$ for *any* continuous bounded function on $\mathbb{R}^n$ and not just those going to a constant at ∞. In particular, $\int e^{ixy}\, d\mu_\infty(y) = 1$ for $|x|$ small. Let Q be the family of points in this set of small x, all of whose coordinates are rational. It is easy to see that $\bigcap_{x \in Q} \{y \,|\, e^{ixy} = 1\} = \{0\}$ so we conclude that $\mu_\infty = \delta_0$, the point mass at zero. Since every limit point of μ_m is δ_0, $\mu_m \to \delta_0$ weakly, and as above $\int f(y)\, d\mu_m(y) \to f(0)$ for any continuous bounded f. In particular, $G_m(x) \to 1$ for all x. ∎

XIII.13 Absence of positive eigenvalues

We have thus far avoided discussing the question of whether Schrödinger operators can have eigenvalues embedded in the continuous spectrum. This question turns out to be very difficult; the results that do exist generally require more detailed assumptions than for any other spectral problem. Moreover, the problem is especially frustrating since one has good physical reasons, which we discuss below, for expecting that such eigenvalues should not occur. Let us consider the intuition behind a simple case. Consider a potential $V(x)$ that goes to zero as $|x| \to \infty$. Classically, the only way to

prevent a particle of positive energy from reaching infinity is to put up a barrier, i.e., trap it by energy conservation. But quantum mechanically, there is tunneling through barriers, so one would guess that a positive energy bound state cannot occur. This guess is wrong!

Example 1 (the Wigner–Von Neumann potential) To find a potential V so that there is a square integrable ψ with $(-\Delta + V)\psi = \psi$, we try to guess ψ. If u is spherically symmetric and $u(r) = r\psi(r)$, then $-u'' + Vu = u$ or $V = 1 + u''u^{-1}$. For V to go to zero at infinity, $u''u^{-1}$ has to go to -1 at infinity, which suggests that we try the ansatz $u(r) = (\sin r)w(r)$. Then

$$V(r) = w''(r)w(r)^{-1} + 2(\cot r)w'(r)w(r)^{-1}$$

For V to be nonsingular, we need w' to vanish whenever $\sin r$ does. Thus w must behave something like

$$g(r) = 2r - \sin 2r = 4\int_0^r \sin^2 x\, dx \tag{85}$$

Of course, if we take $w = g$, then u will not be square integrable. But if we take $w = (1 + g(r)^2)^{-1}$, then w will be square integrable and $w' = -2g'g \times (1 + g^2)^{-2}$ will have zeros in the right places. Making this choice of w, we compute V and find

$$V(r) = [1 + g(r)^2]^{-2}(-32 \sin r)[g(r)^3 \cos r - 3g(r)^2 \sin^3 r + g(r)\cos r + \sin^3 r]$$

where $g(r)$ is given by (85). This rather complicated V has the property that $-\Delta + V$ has an eigenvalue at $+1$ with eigenvector

$$\psi(r) = (r^{-1} \sin r)(1 + g(r)^2)^{-1}$$

even though V is bounded and $V \to 0$ at infinity so that $[0, \infty) \subset \sigma(-\Delta + V)$ by Weyl's essential spectrum theorem. Notice that V has the asymptotic behavior

$$V(r) = -8 \sin 2r/r + O(r^{-2})$$

That is, V oscillates and falls off slowly at ∞. We shall see that both these features are critical for positive eigenvalues to occur. Further discussion of this kind of example can be found in the second and third appendices to Section XI.8.

The physicist confident in the prediction that positive eigenvalues cannot occur must confront Example 1 and answer the question: Why is the intuition wrong? The critical aspect of V is its oscillations. As in Example 1 in the

Appendix to Section X.1, we have used the fact that quantum-mechanical particles are reflected off bumps. The potential V is constructed in such a way that for a particular standing wave pattern these reflections occur coherently. This interpretation suggests that the occurrence of positive energy eigenvalues is a very unusual thing depending on detailed "coherence" properties in the potential. It also indicates that it will be difficult to formulate simple general conditions that exclude the possibility of such bound states.

Example 2 Let $V(x) = \big||x| - 1\big|^{-1}$ on $\mathbb{R}^3$. V is not even in $L^1_{1\text{oc}}(\mathbb{R}^3)$, but $Q(V) \cap Q(-\Delta)$ is dense and so $-\Delta + V$ can be defined as a sum of quadratic forms. This operator will have positive energy eigenvalues for a simple reason: Any $\psi \in Q(V) \cap Q(-\Delta)$ will vanish on the sphere of radius 1 in a suitable sense and so $-\Delta + V$ will leave $\mathscr{H}_1 = L^2(\{x \,|\, |x| \leq 1\})$ invariant. Thus $\mathscr{H}$ will decompose into a direct sum $\mathscr{H}_1 \oplus \mathscr{H}_2$ so that $H = H_1 \oplus H_2$ and H_1 will have purely discrete spectrum. The proofs of these assertions are left to the reader (Problem 104).

This example is rather artificial, but it does show that the question of positive eigenvalues is connected with the question of whether $-\Delta + V$ can have eigenvectors with compact support. We return to this aspect of the question below and in the appendix.

Example 3 Let V be a spherical square well on $\mathbb{R}^3$, $V(x) = -c$ if $|x| \leq 1$, and $V(x) = 0$ if $|x| > 1$. We seek solutions of $(-\Delta + V)\psi = 0$. If $\psi(x) = |x|^{-1}u(|x|)Y_{\ell m}(\hat{x})$ where $\hat{x}$ is the unit vector in direction x and $Y_{\ell m}$ is a spherical harmonic, then u obeys

$$-u'' + \ell(\ell+1)r^{-2}u + V(r)u = 0 \tag{86}$$

The solutions of (86) in the region $r > 1$ where $V = 0$ are $r^{-\ell}$ and $r^{\ell+1}$. If the solution of (86) that is regular at $r = 0$ is pure $r^{-\ell}$ in the region $r > 1$ (and this will occur as c is varied) and $\ell \geq 1$, then $(-\Delta + V)\psi = 0$ will have square integrable solutions.

This example illustrates that zero energy eigenvalues, and more generally threshold eigenvalues in n-body systems, are perfectly normal occurrences that we cannot hope to eliminate.

Example 4 Consider the helium atom Hamiltonian

$$H(\beta) = -\Delta_1 - \Delta_2 - 2|r_1|^{-1} - 2|r_2|^{-1} + \beta|r_1 - r_2|^{-1}$$

which we have discussed extensively in Section XII.6. When $\beta = 0$, we found a high multiplicity of eigenvalues in the continuum. This was because states with the proper energy to decay could not decay because decay would involve the transfer of energy from one particle to another and such transfer cannot occur when $\beta = 0$ because the two particles do not interact with each other. Even when $\beta \neq 0$, there remained eigenvalues embedded in the continuum because of an underlying symmetry, namely, "naturalness" of parity. Notice that all these embedded eigenvalues occur at negative energies.

The moral of the above example is that it should be especially difficult to prove that n-body Schrödinger operators have no embedded eigenvalues at negative energies. In the above cases, there is a simple reason that such eigenvalues occur. But given an n-body system, how does one express the fact that there are no "hidden" symmetries that could produce embedded eigenvalues?

With the examples in mind, it is clear why the problem at hand is so difficult. One has an intuition that positive energy eigenvalues do not occur in "reasonable" situations, but it is clear that such eigenvalues can occur due to "unreasonable" subtleties. We shall present four rather different approaches to the problem. The first is for the two-body central case. In this case, the Schrödinger equation can be formally reduced to an ordinary differential equation, so it is fairly easy to obtain results. We do not attempt to give the strongest conditions involving local singularities.

Theorem XIII.56 Let V be a spherically symmetric function on $\mathbb{R}^n$ with

$$\int_a^\infty |V(r)|\, dr < \infty \tag{87}$$

for some $a > 0$. Suppose that $V \in L^2_{1oc}(\mathbb{R}^n \backslash 0)$ and let H be any self-adjoint extension of $-\Delta + V$ on $C_0^\infty(\mathbb{R}^n \backslash 0)$ that commutes with rotations. Then H has no strictly positive eigenvalues.

Proof Suppose that $(-\Delta + V)\psi = E\psi$. Expand ψ in a partial wave (spherical harmonic) expansion. Then some partial wave component is non-zero, and so we have a distributional solution of

$$-u'' + cr^{-2}u + Vu = Eu \tag{88}$$

on $(0, \infty)$ that is square integrable. Here c is a constant depending on the partial wave index. As in Section XI.8, since $E > 0$, we can find two independent Jost solutions of the integral equation associated to (88) because of the

condition (87). It is not difficult (Problem 105) to show that any solution of (88) must be a linear combination of these two Jost solutions. Since no such linear combination is square integrable at infinity, u must be identically zero. ∎

While the potential of Example 1 fails to obey (87), it is precisely of the form discussed in the appendix to Section XI.8 where we constructed Jost solutions for potentials of the form

$$V(x) = \sum_{i=1}^{N} c_i r^{-1} \sin(\alpha_i r) + O(r^{-1-\varepsilon})$$

for any $k^2 \neq 0, \frac{1}{4}\alpha_1^2, \ldots, \frac{1}{4}\alpha_N^2$. Thus, by the above argument, we see that the Wigner–Von Neumann potential can have a positive eigenvalue only at energy one, the energy at which it does have such a bound state.

Our next result will allow potentials that are not spherically symmetric. One important element of the method involves a "unique continuation theorem for Schrödinger operators." To see how such a result enters suppose that $V \in C_0^\infty(\mathbb{R}^3)$ with supp $V \subset \{x \,|\, |x| < R\}$. If $(-\Delta + V)u = Eu$, then u obeys $-\Delta u = Eu$ on $\{x \,|\, |x| > R\} = \Omega$. As above, we can expand u in a spherical harmonic expansion in Ω, and so conclude that $u = 0$ on Ω. To conclude that u is identically zero we need:

Theorem XIII.57 Let V be a function on $\mathbb{R}^n$ so that:

(i) Multiplication by V is $-\Delta$-bounded with relative bound less than 1.
(ii) There is a closed set S of measure zero so that $\mathbb{R}^n \backslash S$ is connected and so that V is bounded on any compact subset of $\mathbb{R}^n \backslash S$.

Let $H = -\Delta + V$ and suppose that $Hu = Eu$ for some E and $u \in L^2$. Suppose that u vanishes on some open subset of $\mathbb{R}^n$. Then u is identically zero.

As the proof in the appendix shows, this result is really a local result dealing with distributional solutions of $(-\Delta + V)u = Eu$ which are locally in $D(-\Delta)$. The reason for hypothesis (i) is just to ensure that eigenfunctions are locally in $D(-\Delta)$.

The above proves that $\sigma_p(-\Delta + V) \cap (0, \infty) = \varnothing$ for $V \in C_0^\infty$. This is a special case of the following general result:

Theorem XIII.58 (Kato–Agmon–Simon theorem) Suppose that V is a potential satisfying the hypothesis of Theorem XIII.57 and that, in addition, $V = V_1 + V_2$ where:

(i) V_1 is bounded outside some ball $\{x \,|\, |x| < R_0\}$, and $|x| V_1(x) \to 0$ as $|x| \to \infty$.

(ii) V_2 is bounded outside some ball, $\{x \mid |x| < R_0\}$, and $V_2(x) \to 0$ as $|x| \to \infty$.

(iii) If we consider V_2 as a map $r \mapsto V_2(r, \cdot)$ from $(0, \infty)$ to $L^\infty(S^{n-1})$ where S^{n-1} is the $(n-1)$-dimensional sphere, then for $|x| > R_0$, V_2 is differentiable as an L^∞-valued function and $\overline{\lim}_{r\to\infty} r\, \partial V_2/\partial r \leq 0$.

Then, $H = -\Delta + V$ has no strictly positive eigenvalues.

Proof Consider the alternative hypotheses:

(ii′) $V_2(x) < 0$ for $|x| > R_0$ replaces $V_2(x) \to 0$.
(iii′) $\partial V_2(x)/\partial r \leq -r^{-1} V_2$ for $|x| > R_0$ replaces $\lim_{r\to\infty} r\, \partial V_2/\partial r \leq 0$.

Suppose that we can show that $-\Delta + V$ has no strictly positive eigenvalues assuming (i), (ii′), (iii′). Given V_2 obeying (ii) and (iii), the function $\tilde{V}_2 = V_2 - \varepsilon$ obeys (ii′) and (iii′), at least if R_0 is taken sufficiently large. Applying the putative (i)–(iii′) result to $-\Delta + V_1 + \tilde{V}_2$ we see that $-\Delta + V$ has no eigenvalues in (ε, ∞). Since ε is arbitrary, we can complete the proof of the theorem. Thus we suppose that (i), (ii′), (iii′) hold.

Suppose that ψ is a real eigenfunction for $-\Delta + V$ with eigenvalue $E > 0$. Define a function w from $(0, \infty)$ to $L^2(S^{n-1}, d\Omega)$ by

$$w(r, \Omega) = r^{(n-1)/2} \psi(r\Omega) \tag{89}$$

so that

$$\int_0^\infty \|w(r)\|^2_{L^2(S^{n-1},\, d\Omega)}\, dr < \infty$$

From now on we drop the subscript on the norm. More generally, given any $\varphi \in L^2(\mathbb{R}^n)$, define $w_\varphi \in L^2((0, \infty); L^2(S^{n-1}, d\Omega), dr)$ by (89) with ψ replaced by φ. If $\varphi \in C_0^\infty(\mathbb{R}^n)$, then

$$w_{H\varphi} = -w_\varphi'' - r^{-2} B w_\varphi + \tfrac{1}{4}(n-1)(n-3) r^{-2} w_\varphi + V w_\varphi \tag{90}$$

where B is the Laplace–Beltrami operator on $L^2(S^{n-1})$ described in Example 4 of the Appendix to Section X.1. (90) can be proven by using a spherical harmonic expansion as in that example. Below, we only need to know that $-B$ is a positive operator.

In terms of the function w of (89), define for $r > R_0$,

$$F(r) = (w', w') + r^{-2}(w, Bw) + (w, (E - V_2(r))w) \tag{91}$$

where all inner products are in $L^2(S^{n-1}, d\Omega)$. The objects occurring in (91) are all well defined, for one first notes that for $\varphi \in C_0^\infty$,

$$\int_0^\infty [(\dot{w}_\varphi, \dot{w}_\varphi) - r^{-2}(w_\varphi, Bw_\varphi)]\, dr = \|\nabla\varphi\|^2_{L^2(\mathbb{R}^n)}$$

where $\dot{w}_\varphi = r^{(n-1)/2}(d/dr)(r^{-(n-1)/2}w_\varphi)$. From this estimate it follows that w'_φ and (w_φ, Bw_φ) are defined almost everywhere on $(0, \infty)$ if $\varphi \in Q(-\Delta)$.

Choose $R_1 > R_0$ so that

$$|rV_1(r)| + \tfrac{1}{4}(n-1)(n-3)r^{-1} < k \equiv \sqrt{E}$$

for $r > R_1$. Such an R_1 exists by hypothesis (i). We claim that almost everywhere

$$F(r) \geq r^{-1}r_1 F(r_1), \qquad r > r_1 > R_1 \tag{92}$$

Let us first give a formal proof of (92). Formally, if $r > R_1$,

$$\begin{aligned}\frac{d}{dr}(rF(r)) &= 2r(w', w'' + r^{-2}Bw + (E - V_2)w) \\ &\quad + \|w'\|^2 - r^{-2}(w, Bw) + E\|w\|^2 - (w, (rV_2)'w) \\ &\geq 2(w', (rV_1 + \tfrac{1}{4}(n-1)(n-3)r^{-1})w) + \|w'\|^2 + E\|w\|^2 \\ &\geq 0\end{aligned}$$

where the first inequality follows from the (formal) eigenfunction relation and the facts that $-B$ is positive and that $(rV_2)' = rV_2' + V_2 \leq 0$ by hypothesis (iii′). The final inequality comes from the choice of R_1. Of course, (92) comes from integrating this inequality.

Now we give a rigorous proof of (92). Let $\varphi \in C_0^\infty$ and define F_φ by (91) with w_φ replacing w. The differentiations done formally above on F are legitimate on F_φ and imply that

$$\frac{d}{dr}(rF_\varphi) \geq 2r(w'_\varphi, (Ew_\varphi - w_{H\varphi}))$$

for $r > R$. Therefore, if $r > r_1 > R_1$, we have

$$rF_\varphi(r) \geq r_1 F_\varphi(r_1) + \int_{r_1}^{r} 2t(w'_\varphi(t), Ew_\varphi(t) - w_{H\varphi}(t))\,dt$$

Now pick $\varphi_n \in C_0^\infty$ so that $\varphi_n \to \psi$ and $-\Delta\varphi_n \to -\Delta\psi$ (such a choice is possible since C_0^∞ is a core for $-\Delta$). Then $H\varphi_n \to H\psi = E\psi$. Thus, $w_{\varphi_n} \to w$, $w_{H\varphi_n} \to Ew$, and $w'_{\varphi_n} \to w'$ in $L^2((0, \infty); L^2(S^{n-1}, d\Omega), dr)$ and, after passing to a subsequence, $F_{\varphi_n} \to F$ pointwise a.e. This proves (92).

From (92) we deduce that $F(r) \leq 0$ for $r > R_1$ because if this were not so, then the left-hand side of (91) would not be integrable. But it is integrable since $\psi \in D(-\Delta)$ (Problem 110). We now want to prove that $w = 0$ for $r > R_2$ for suitable R_2. This will imply that ψ vanishes outside some sphere and so, by the unique continuation theorem, ψ is identically zero. In our

considerations below, we shall only make "formal" computations, leaving it to the reader to supply the arguments analogous to the F_φ argument we have just given.

For any $m \geq 0$, let $w_m = r^m w$ and let

$$G(m, r) = \|w_m'\|^2 + (k^2 - k^2 R_1 r^{-1} + m(m+1)r^{-2})\|w_m\|^2 + r^{-2}(w_m, Bw_m) - (w_m, V_2(r)w_m)$$

Notice first that w_m obeys

$$w_m'' - 2mr^{-1}w_m' + r^{-2}[m(m+1) - \tfrac{1}{4}(n-1)(n-3) + B]w_m + (k^2 - V)w_m = 0$$

Then, using the inequality

$$-(r^2 V_2)' = -r^1 V_2 - r(rV_2)' \geq 0$$

one easily computes that for $r > R_0$,

$$\frac{d}{dr}(r^2 G(m, r)) \geq 2r\left[(2m+1)\|w_m'\|^2 + k^2\left(1 - \frac{R_1}{2r}\right)\|w_m\|^2 + (w_m', (rV_1 + \tfrac{1}{4}(n-1)(n-3)r^{-1} - k^2 R_1)w_m)\right]$$

Thus, for $r > R_1$,

$$\frac{d}{dr}(r^2 G(m, r)) \geq 2r\left[(2m+1)\|w_m'\|^2 + \frac{1}{2}k^2\|w_m\|^2 - (k + k^2 R_1)\|w_m'\|\,\|w_m\|\right]$$

It follows that for some m_0, $r^2 G(m, r)$ is monotone increasing on (R_1, ∞) if $m > m_0$.

Suppose now that $w(r_0) \neq 0$ for some $r_0 > R_1$. Writing

$$G(m, r) = r^{2m}[\|w' + mr^{-1}w\|^2 + (k^2 - k^2 R_1 r^{-1} + m(m+1)r^{-2})\|w\|^2 - (w, V_2 w) + r^{-2}(w, Bw)] \tag{93}$$

we see that $G(m, r_0) > 0$ for m sufficiently large. Combining this with the monotonicity proven above, we conclude: If $w(r_0) \neq 0$ for some $r_0 > R_1$, then for some M (depending on r_0) $G(m, r) > 0$ for all $m > M$, $r > r_0$.

Now we can complete the proof. Given r_0 with $w(r_0) \neq 0$ and $r_0 > R_1$, choose $m_0 > M$ and then $R_2 > r_0$ so that for $r > R_2$,

$$-k^2 R_1 r^{-1} + m_0(2m_0 + 1)r^{-2} < 0$$

Since $\int_{R_2}^{\infty} \|w\|^2 \, dr < \infty$, $\|w\|$ is not strictly monotone increasing on all of $[R_2, \infty)$ and so there is some $r_1 > R_2$ so that

$$\frac{d}{dr} \|w\|^2 \Big|_{r=r_1} = 2(w', w) \leq 0$$

In particular, at $r = r_1$,

$$\|w' + mr^{-1}w\|^2 \leq \|w'\|^2 + m^2 r^{-2} \|w\|^2$$

so by (93)

$$0 < r_1^{-2m_0} G(m_0, r_1) \leq \|w'\|^2 + k^2 \|w\|^2 - (w, V_2 w) + r^{-2}(w, Bw) = F(r_1)$$

Given (92), this implies that $\int \|w\|^2 \, dr = \infty$ or $\|w\|^2 = 0$, so $w(r_0) = 0$ for all $r_0 > R_1$. By unique continuation (Theorem XIII.57), ψ is identically zero. ∎

Corollary Suppose that V satisfies the hypotheses of Theorem XIII.57. If V has compact support or if V is repulsive near ∞ ($\partial V/\partial r \leq 0$), then there are no bound states of positive energy.

Notice that because of its asymptotic behavior, the potential of Example 1 fails both the $rV_1 \to 0$ condition and the $r \, \partial V_2/\partial r$ condition.

The third method for controlling positive energy bound states that we shall discuss involves the virial theorem. This theorem asserts that if ψ is an eigenfunction of $H = -\Delta + V$, then under suitable hypotheses on V:

$$2(\psi, (-\Delta)\psi) = (\psi, \mathbf{r} \cdot \nabla V \psi) \tag{94}$$

(94) is clearly a useful tool in studying bound states. For example, if $\mathbf{r} \cdot \nabla V \leq 0$ (which is an expression of the fact that V is repulsive), then clearly H can have no bound states since then the right-hand side of (94) would always be negative and the left strictly positive. Formally, (94) comes from the following argument. Let

$$D = \frac{in}{2} + i \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i}$$

Then

$$i[D, H] = 2(-\Delta) - \mathbf{r} \cdot \nabla V$$

so that if ψ is an eigenfunction with eigenvalue E,

$$\begin{aligned} 2(\psi, -\Delta\psi) - (\psi, \mathbf{r} \cdot \nabla V) &= (\psi, i[D, H]\psi) \\ &= -iE\{(\psi, D\psi) - (\psi, D\psi)\} \\ &= 0 \end{aligned}$$

since H is Hermitian. This argument is only formal since D is an unbounded operator and ψ need not be in its domain. In fact, there are modifications of the potential in Example 1 which have eigenfunctions that are not in the domain of D (Problem 107)! The key to our proof of the virial theorem is the realization that the group generated by D is the group of dilations discussed in Section 10. For $a > 0$, define the unitary family

$$(U_a\psi)(x) \equiv (e^{-iD\log a}\psi)(x) = a^{n/2}\psi(ax)$$

and set

$$V_a(x) = V(ax)$$

so that $V_a = U_a V U_a^{-1}$ for a multiplication operator V.

Theorem XIII.59 (the virial theorem) Suppose that V is a multiplication operator on $L^2(\mathbb{R}^n)$ and that:

(i) V is $-\Delta$-bounded with relative bound less than one.
(ii) There is a multiplication operator W on $L^2(\mathbb{R}^n)$ with $D(W) \supset D(-\Delta)$ so that for all $\psi \in D(-\Delta)$,

$$(a-1)^{-1}(V_a - V)\psi \to W\psi \qquad \text{as} \quad a \to 1 \tag{95}$$

Then if $\psi \in D(-\Delta)$ and $-\Delta\psi + V\psi = E\psi$, we have

$$2(\psi, -\Delta\psi) = (\psi, W\psi) = 2(\psi, (E - V)\psi) \tag{96}$$

Proof Since $U_a(-\Delta)U_a^{-1} = a^{-2}(-\Delta)$, we have

$$(-\Delta + a^2 V_a)\psi_a = a^2 E\psi_a$$

as well as $(-\Delta + V)\psi = E\psi$. These two relations imply that

$$\begin{aligned} E(a^2-1)(\psi_a, \psi) &= ((-\Delta + a^2V_a)\psi_a, \psi) - (\psi_a, (-\Delta + V)\psi) \\ &= a^2(V_a\psi_a, \psi) - (\psi_a, V\psi) \end{aligned}$$

since $-\Delta$ is symmetric. Thus

$$(a+1)(\psi_a, V_a\psi) + (a-1)^{-1}(\psi_a, (V_a - V)\psi) = E(a+1)(\psi_a, \psi)$$

Taking the limit as $a \to 1$ yields (96). ∎

We remark that formally W is just $\mathbf{r} \cdot \nabla V$. In fact, since $C_0^\infty(\mathbb{R}^n) \subset D(-\Delta)$, if (95) holds, W is given by $\mathbf{r} \cdot \nabla V$ where the derivatives are interpreted in the sense of distributions. Secondly, (95) is typically proven in the following way: Suppose that $(a-1)^{-1}(V_a - V)$ converges pointwise to a function W and that there is a multiplication operator $\tilde{W}$ with $D(\tilde{W}) \supset D(-\Delta)$ so that

$$|(a-1)^{-1}(V_a - V)| \le \tilde{W}$$

pointwise a.e. for a close to one. Then $D(W) \supset D(-\Delta)$ and the dominated convergence theorem allows one to conclude (95).

Theorem XIII.60 Let V be a real-valued function that is $-\Delta$-bounded with relative bound less than one. Then $-\Delta + V$ has no positive eigenvalues if at least *one* of the following conditions holds:

(i) V satisfies the hypotheses of Theorem XIII.59 and V is repulsive (that is, $V(ar) \leq V(r)$ for all r and all $a > 1$).

(ii) V is homogeneous of degree $-\alpha$ where $0 < \alpha < 2$ (that is, $V(ar) = a^{-\alpha}V(r)$).

(iii) V satisfies the hypotheses of Theorem XIII.59 and for some $b > 0$ we have

$$-\Delta - \tfrac{1}{2}(1 + b)W - bV \geq 0 \tag{97}$$

Proof If (ii) holds, then it is easy to check that the hypotheses of Theorem XIII.59 hold. So, in all three cases let W be as in Theorem XIII.59. Then

$$(\psi, -\Delta\psi) = \tfrac{1}{2}(\psi, W\psi)$$

for any eigenfunction ψ. In case (i), $W(x) \leq 0$ so $\psi = 0$ since $H_0 \geq 0$ and $\mathrm{Ker}(H_0) = \{0\}$. In case (ii), $W = -\alpha V$, so by (96),

$$\begin{aligned} 2E(\psi, \psi) = (2 - \alpha)(\psi, V\psi) &= -\alpha^{-1}(2 - \alpha)(\psi, W\psi) \\ &= -2\alpha^{-1}(2 - \alpha)(\psi, H_0\psi) \end{aligned}$$

Since $2 - \alpha > 0$ and $-\Delta \geq 0$, we conclude that $E < 0$. Finally, in case (iii), for any eigenfunction ψ, we have

$$\begin{aligned} -bE(\psi, \psi) &= -b(\psi, (H_0 + V)\psi) + (1 + b)(\psi, (H_0 - \tfrac{1}{2}W)\psi) \\ &= (\psi, [H_0 - \tfrac{1}{2}(1 + b)W - bV]\psi) \end{aligned}$$

so that (97) implies that $E \leq 0$. ∎

We emphasize that the potentials in this theorem are not required to go to zero at infinity, so the theorem can be applied to many-body Schrödinger operators.

Example 5 (Coulomb systems, including atomic Hamiltonians) Suppose that we have an n-body system with two body forces that are all of the form $a_{ij}|r_i - r_j|^{-1}$. Then V is homogeneous of degree -1, so by (ii) of Theorem XIII.60, $H = -\Delta + V$ has no positive eigenvalues.

Example 6 Let us illustrate (iii) of Theorem XIII.60 by a simple example. Let $V \in C_0^\infty(\mathbb{R}^n)$ with $n \geq 3$. We have seen in Section 3 that $-\Delta + \lambda V$ has no negative eigenvalues so long as λ is sufficiently small. What about positive eigenvalues? The smoothness techniques of Section 7 imply that there are no positive eigenvalues either. And, Theorem XIII.58 says that there are no positive eigenvalues for any value of λ. An alternative proof is available for small λ, since $-\mathbf{r} \cdot \nabla V - V$ is also in $C_0^\infty(\mathbb{R}^n)$. Thus, for λ small $-\Delta - \lambda(\mathbf{r} \cdot \nabla V + V)$ has no negative eigenvalues and so is a positive operator. It follows from part (iii) of Theorem XIII.60 that $-\Delta + \lambda V$ has no positive eigenvalues for λ small.

Theorem XIII.60 does not exhaust the information available from the virial theorem. For example, one can deal with sums of potentials of the type considered there (Problem 108). For some potentials one can prove the absence of eigenvalues in some interval (a, ∞) with $a > 0$.

Example 7 Let

$$H = -\sum_{j=1}^{n} \Delta_j + \sum_{j=1}^{n} V_j(\mathbf{r}_j) + \sum_{i<j} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

on $L^2(\mathbb{R}^{3n})$ where $V_j(\mathbf{r}_j) = -b_j r_j^{-1} \exp(-a_j r_j)$ and

$$V_{ij}(\mathbf{r}) = b_{ij} r^{-1} \exp(-a_{ij} r)$$

with all a and b positive constants. Let $U(r) = r^{-1}(\exp(-ar))$. Then $r\, dU/dr = -U - a \exp(-ar)$ so that if $V = \sum_{j=1}^{n} V_j + \sum_{i<j} V_{ij}$, then

$$\mathbf{x} \cdot \nabla V + V \leq \sum_{j=1}^{n} a_j b_j$$

It follows that, if $(-\Delta + V)\psi = E\psi$, then

$$E(\psi, \psi) = -(\psi, H_0 \psi) + (\psi, (\mathbf{x} \cdot \nabla V + V)\psi)$$

$$\leq \sum_{j=1}^{n} a_j b_j (\psi, \psi)$$

so that H has no eigenvalues in $(\sum_{j=1}^{n} a_j b_j, \infty)$.

There is a connection between virial theorem methods and the result of Theorem XIII.58. For example, if V is negative for all x and homogeneous of degree $-\alpha$ with $\alpha \leq 1$, then near infinity the conditions (ii′) and (iii′) of the proof of Theorem XIII.58 hold, so we can conclude that $-\Delta + V$ has no positive eigenvalues by either method. The distinction between the types of

results is that Theorem XIII.58 requires only information at infinity, while Theorem XIII.60 requires global hypotheses.

There is also a connection between virial theorem methods and our final method. The role played by dilations in the above suggests the dilation analytic methods of Section 10 might be relevant to the problem of positive energy bound states. To see that they are, let us first reconsider the case of Coulomb potentials:

Example 5, revisited Let H be the Hamiltonian of an n-body system whose two body potentials are all homogeneous of some fixed degree $-\alpha$ where $0 < \alpha < 1$. Then the potentials are all dilation analytic, in fact,

$$U(\theta)VU(\theta)^{-1} = e^{-\alpha\theta}V$$

where $U(\theta)$ is the group of dilations of Section 10. Suppose that E_0 is the largest threshold of $H_0 + V$ (we will eventually prove that $E_0 = 0$) and that $E > E_0$ is an eigenvalue of H. By our general analysis of dilation analytic Hamiltonians, $H(\theta)$ will have E as a discrete eigenvalue so long as $0 < \text{Im } \theta < \pi$. Writing

$$H(\theta) = e^{-2\theta}(H_0 - e^{-(\alpha-2)(\theta-\theta_0)}V)$$

with $\theta_0 = i\pi/(2-\alpha)$, we note that

$$H(\theta_0) = e^{-2\theta_0}(H_0 - V)$$

so that any eigenvalues of $H(\theta_0)$ must have argument $2i\theta_0 \neq 0$ or $\pi + 2i\theta_0 \neq 0$. Thus E cannot be an eigenvalue of $H(\theta_0)$ and so of H (see Figure XIII.6a). The condition $\alpha < 1$ is needed to ensure that $\text{Im } \theta_0 < \pi$.

Now by induction we claim that $E_0 = 0$, for this is true in the two-body system and clearly if it is true in all k-body systems with $k < n$, then by the above argument all k-body systems with $k < n$ have no positive eigenvalues and so the n-body system has no positive thresholds. Notice that by the above argument we can actually prove that $H(\theta)$ has no eigenvalues in $\{E \,|\, 0 \leq \arg E < 2 \text{ Im } \theta\}$, for $0 > \text{Im } \theta > -\pi$.

Now let V be a Coulomb potential. Let V_α be the potential obtained by replacing $|r_i - r_j|^{-1}$ by $|r_i - r_j|^{-\alpha}$. By analytic perturbation theory, if $H_0 + V$ has a positive eigenvalue, then for, say $\theta = -i\pi/3$, $H_0(\theta) + V_\alpha(\theta)$ will have an eigenvalue near the positive real axis for $\alpha - 1$ small. But, by general principles, this eigenvalue cannot have small negative argument for α real. By the above argument, for α real and less than 1, it cannot have argument zero or small and positive. This contradiction shows that $H_0 + V$ cannot have any positive eigenvalues (see Figure XIII.6b).

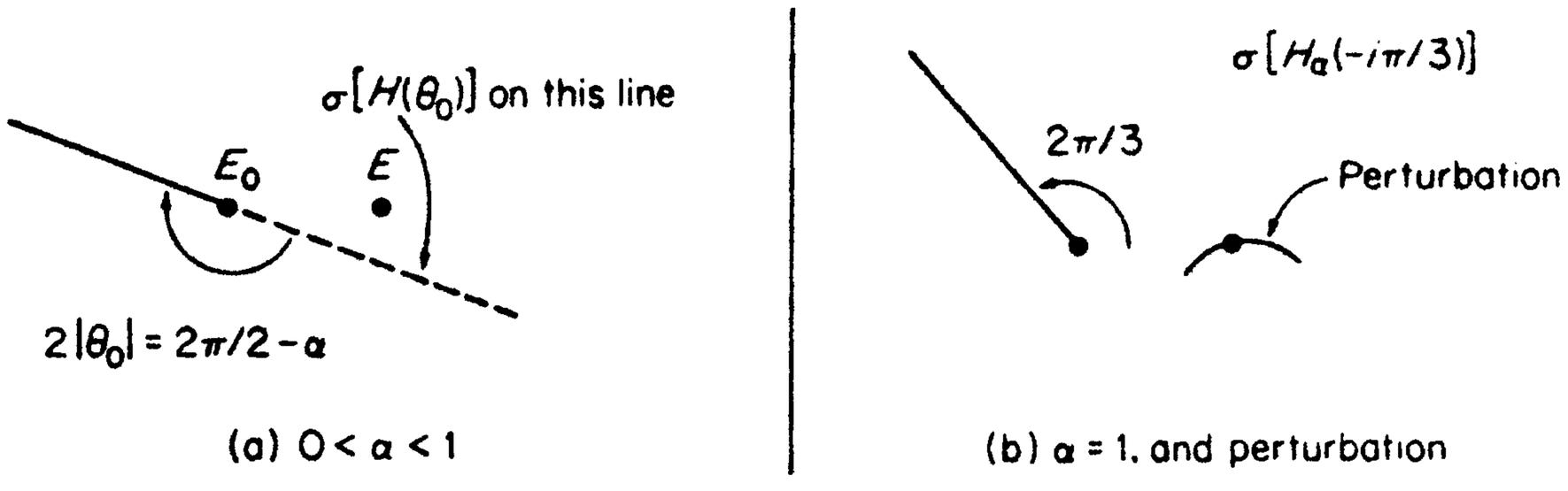


FIGURE XIII.6

Example 5 (revisited, alternative argument) There is another way of obtaining the results we have just discussed that allows $0 < \alpha < 2$ and which also requires all potentials to be homogeneous of the same degree. $H_0(\theta) = e^{-2\theta}H_0$, $V(\theta) = e^{-\alpha\theta}V$. Thus for any $\varphi \in Q(H_0)$, $(\varphi, H_0(\theta)\varphi)$ has argument $2\pi - 2 \operatorname{Im}\theta$ while $(\varphi, V(\theta)\varphi)$ has argument $2\pi - \alpha \operatorname{Im}\theta$ or $\pi - \alpha \operatorname{Im}\theta$. Thus, since $\alpha < 2$, $(\varphi, H(\theta)\varphi)$ has argument between $\pi - \alpha \operatorname{Im}\theta$ and $2\pi - \alpha \operatorname{Im}\theta$ for $\operatorname{Im}\theta$ small and positive. In particular, $(\varphi, H(\theta)\varphi)$ cannot have argument zero and so $H(\theta)\varphi$ cannot be $E\varphi$ with $E > 0$. Since $H(\theta)$ cannot have positive eigenvalues, neither can H.

There is one especially interesting feature of the above argument: There is a distinction between positive and negative eigenvalues, as there must be due to Example 4; the distinction occurs at $\operatorname{Im}\theta = \pm\frac{1}{2}\pi$. For $|\operatorname{Im}\theta| < \frac{1}{2}\pi$, any eigenvalue of H at a nonthreshold point is a discrete eigenvalue of $H(\theta)$. As $\operatorname{Im}\theta$ approaches $\pm\frac{1}{2}\pi$, the continuous spectrum approaches the negative eigenvalues, so we cannot assert that the eigenvalues remain for $\operatorname{Im}\theta > \frac{1}{2}\pi$ (and in particular, for $\theta = \theta_0$). But positive eigenvalues stay away from the continuous spectrum for $|\operatorname{Im}\theta| \in (0, \pi)$. This distinction suggests that dilation analytic potentials allowing a continuation up to $\operatorname{Im}\theta = \frac{1}{2}\pi$ might be special. We therefore define:

Definition We say that a "potential" V lies in $\mathscr{F}_{\pi/2}$ if and only if:

(1) V is a quadratic form with form domain $D(-\Delta)$.
(2) $(-\Delta + 1)^{-1/2}[U(\theta)VU(\theta)^{-1}](-\Delta + 1)^{-1/2}$ defined as an operator for $\theta \in \mathbb{R}$ is the restriction to the real axis of a compact operator-valued function that is analytic in the strip $|\operatorname{Im}\theta| < \frac{1}{2}\pi$ and norm continuous in the strip $|\operatorname{Im}\theta| \leq \frac{1}{2}\pi$.

As we shall see, $\mathscr{F}_{\pi/2}$ includes the Coulomb and Yukawa potentials. We shall prove presently that any N-body system all of whose two-body potentials lie in $\mathscr{F}_{\pi/2}$ has no positive eigenvalues. To do this, we need a complex variables theorem related to Theorem XII.18.

Lemma (Carlson's theorem) Suppose that f is a complex-valued function defined and continuous in $\{z \mid \text{Re } z \geq 0\}$ and analytic in $\{z \mid \text{Re } z > 0\}$. Suppose that

$$|f(z)| \leq Me^{A|z|} \qquad \text{all } z \text{ with Re } z \geq 0 \tag{98a}$$

$$|f(iy)| \leq Me^{-B|y|} \qquad \text{all } y \in \mathbb{R} \tag{98b}$$

where $B > 0$. Then f is identically zero.

Proof Let us first prove a slightly strengthened version of the maximum principle called the **Phragmen–Lindelöf principle**: Suppose that g is analytic in the wedge

$$N = \{re^{i\theta} \mid r > 0,\ \alpha < \theta < \beta\}$$

and continuous in $\bar{N}$ and that $\beta - \alpha < \pi$. Then if $|g(z)| \leq C_1 \exp(C_2|z|)$ in $\bar{N}$, we have

$$|g(z)| \leq \sup_{y \geq 0} \{|g(ye^{i\alpha})|,\ |g(ye^{i\beta})|\} \equiv D$$

To prove this, we first suppose without loss that $\beta < \frac{1}{2}\pi\mu^{-1}$, $\alpha > -\frac{1}{2}\pi\mu^{-1}$, where $\mu > 1$. Let

$$g_\varepsilon(z) = g(z)\exp(-\varepsilon z^\mu)$$

Then $g_\varepsilon \to 0$ as $|z| \to \infty$ in $\bar{N}$, so, by the ordinary maximum principle, $g_\varepsilon(z)$ takes its maximum on ∂N. Thus

$$|g_\varepsilon(z)| \leq D$$

for any ε. Taking $\varepsilon \downarrow 0$, we see that $|g(z)| \leq D$.

Now suppose that f obeys (98). Let

$$h(z) = f(z)\exp(-iBz - Az)$$

Then $|h(z)| \leq M$ if $|\arg z| = 0$ or $\frac{1}{2}\pi$ and $|h(z)| \leq M\exp((A+B)|z|)$ for all z. Thus, by the Phragmen–Lindelöf principle, $|h(z)| \leq M$ if $0 \leq \arg z \leq \frac{1}{2}\pi$. It follows that

$$|f(z)| \leq M\exp(A|z|\cos\theta - B|z||\sin\theta|); \qquad \theta = \arg z \tag{99}$$

for $0 \leq \theta \leq \frac{1}{2}\pi$ and similarly for $0 \geq \theta \geq -\frac{1}{2}\pi$.

Now consider the function $g(x) = f(ix)$ for x real and let $\hat{g}$ be its Fourier transform. By (99),

$$|g(x - iy)| \leq M\exp(A|y|), \qquad y > 0$$

so a Paley–Wiener argument implies that $\hat{g}(k) = 0$ if $k < -A$. Since

$$|g(x)| \leq M \exp(-\beta|x|)$$

Paley–Wiener arguments also imply that $\hat{g}$ is analytic in a neighborhood of the real axis. It follows that g is identically zero so f is zero also. ∎

Theorem XIII.61 (Balslev–Simon theorem) Let H be an N-body Schrödinger operator on $L^2(\mathbb{R}^{nN-n})$ obtained by removing the center of mass motion from

$$\tilde{H} = -\sum_{i=1}^{N} (2m_i)^{-1}\Delta_i + \sum_{i=j} V_{ij}(r_i - r_j)$$

where each V_{ij} is a form in $\mathscr{F}_{\pi/2}$ which is local (i.e., the form of a multiplication operator) and symmetric. Then H has no eigenvalues in $(0, \infty)$.

Proof As in Example 5 (revisited), if we can prove that H has no eigenvalues in $(0, \infty)$ under the hypothesis that H has no positive thresholds, then by an induction argument, we can prove that H has no positive eigenvalues.

If H has no positive thresholds and $E > 0$ is an eigenvalue, then E is also an eigenvalue of $H(\theta)$ for $|\operatorname{Im}\theta| \leq \frac{1}{2}\pi$ and the projection

$$P(\theta) = -(2\pi i)^{-1} \int_{|\lambda - E| = \varepsilon} (H(\theta) - \lambda)^{-1}\, d\lambda$$

defined for $|\operatorname{Im}\theta| > 0$, is analytic in $|\operatorname{Im}\theta| < \frac{1}{2}\pi$ and equal to the spectral projection $P_{\{E\}}(H)$ for $\theta = 0$. Thus, by O'Connor's lemma (the proposition following Theorem XIII.39), any eigenvector ψ with $H\psi = E\psi$ has the property that $U(\theta)\psi$ extends to a function analytic in $\{\theta \,|\, |\operatorname{Im}\theta| < \frac{1}{2}\pi\} = N$, continuous in $\bar{N}$. Moreover, since E is an isolated eigenvalue of $H(\pm i\frac{1}{2}\pi)$, by the arguments of Section 11, $U(\pm i\frac{1}{2}\pi)\psi$ falls off exponentially in the sense that for some $b > 0$, $e^{br}U(\pm i\frac{1}{2}\pi)\psi \in L^2$.

Heuristically, the argument would proceed as follows: Intuitively, the statement that ψ is dilation analytic means that $\psi(x)$, thought of as a function of $r = |x|$ and $\Omega = x/|x|$, is analytic in r for fixed Ω in the region $\operatorname{Re} r > 0$ with

$$e^{-\frac{1}{2}(nN-n)i\theta}(U(\theta)\psi)(r, \Omega) = \psi(re^{i\theta}, \Omega)$$

$\psi \in L^2$ implies that $\psi(z, \Omega)$ is more or less bounded and $U(\pm i\frac{1}{2}\pi)\psi \in D(e^{br})$ implies that $\psi(z, \Omega)$ falls off exponentially if $\arg z = \pm\frac{1}{2}\pi$. Thus $\psi = 0$ by

Carlson's theorem. This argument does not go through because all our information is L^2, but it is the intuition behind the argument below.

Fix $g \in C_0^\infty(\mathbb{R}^{nN-n}\backslash\{0\})$, a function with support away from zero; say supp $g \subset \{x \,|\, |x| > R\}$. For $z \in (0, \infty)$, define

$$F(z) = z^{nN/2} \int \overline{g(x)}\psi(zx)\, d^{nN-n}x$$

$$= z^{n/2}(g, U(\ln z)\psi)$$

Using this formula, we can extend F to a function analytic in $\{z \,|\, \text{Re } z > 0\}$, continuous in $\{z \,|\, \text{Re } z \geq 0\}$.

Since $U(\theta)$ is unitary for θ real,

$$|F(z)| \leq |z|^{n/2}\|g\| \sup_{|y| \leq \pi/2} \|U(iy)\psi\|$$

for all z with Re $z \geq 0$. Moreover, for β real and positive

$$|F(i\beta)| = \left|\beta^{nN/2} \int \overline{g(x)}\left[U\left(i\frac{\pi}{2}\right)\psi\right](\beta x)\, dx\right|$$

$$= \beta^{n/2} \int_{|x| \geq \beta R} \overline{g(\beta^{-1}x)}\left[U\left(\frac{\pi}{2}i\right)\psi\right](x)\, dx$$

$$\leq e^{-\beta Rb}|\beta|^{nN/2}\|g\| \left\| e^{br}U\left(\frac{\pi}{2}i\right)\psi \right\|$$

and similarly for $F(-i\beta)$. Thus, by Carlson's theorem, $F = 0$ so $(g, \psi) = 0$. Since the functions $g \in C_0^\infty(\mathbb{R}^{nN-n}\backslash\{0\})$ are dense, $\psi = 0$. ∎

Example 7, revisited The potential $V(r) = e^{-ar}/r$ is in $\overline{\mathscr{F}}_{\pi/2}$ with $V_\theta(r) = e^{-\theta}r^{-1}\exp(-ae^\theta r)$. Thus the Hamiltonians of Example 7 have no eigenvalues in $(0, \infty)$. This is an improvement of the virial theorem result. However, there are cases where the virial method gives information while Theorem XIII.61 gives none. For example, if $V(r) = be^{-ar}$ with $b > 0$, then $-\Delta + V$ has no positive eigenvalues by the virial theorem, but V is *not* in $\overline{\mathscr{F}}_{\pi/2}$ since $\exp(-ae^\theta r)$ is not a relatively compact multiplication operator, so $V_\theta(r)$ cannot have a *norm* continuous extension to $\{\theta \,|\, |\text{Im } \theta| = \frac{1}{2}\pi\}$.

Example 8 If each V_{ij} is homogeneous of degree β_{ij} with $0 < \beta_{ij} < 2$. Then $\tilde{H} = -\sum_{i=1}^n \Delta_i + \sum_{i<j} V_{ij}$ has the property that after its center of mass motion is removed, it has no positive energy bound states. This result is not obtainable with virial theorem methods although it is reasonable from the virial theorem point of view.

In the above we have concentrated on Schrödinger operators, but the ideas are applicable in other situations. In our study of acoustical scattering by the Lax–Phillips method (Section XI.11), we needed the following result:

Theorem XIII.62 Let σ and λ be real C^2 functions on $\mathbb{R}^3$ so that $\sigma(x) > 0$, $\lambda(x) > 0$, and such that $\sigma_0 - \sigma(x)$ and $\lambda_0 - \lambda(x)$ have compact support for some constants σ_0 and λ_0. Let H be the self-adjoint operator on $L^2(\mathbb{R}^3)$ obtaining by closing the quadratic form

$$q(f, f) = \int_{\mathbb{R}^3} |\nabla(\lambda f)|^2 \sigma \, dx$$

on $C_0^\infty(\mathbb{R}^3)$. Then H has no eigenvalues.

Proof Clearly, for some $a > 0$, $\sigma(x) \geq a$ for all x. Thus, for $f \in D(H)$,

$$(Hf, f) = q(f, f) \geq a \int_{\mathbb{R}^3} |\nabla(\lambda f)|^2 \, dx \geq 0$$

Thus H cannot have any negative eigenvalues and if $Hf = 0$, then $\lambda f = 0$, which implies that $f = 0$, so zero cannot be an eigenvalue either. It remains to eliminate strictly positive eigenvalues.

Suppose that $E > 0$ and that $Hf = Ef$. Let B_R be a ball of radius R containing the supports of $\sigma_0 - \sigma(x)$ and $\lambda_0 - \lambda(x)$. Then, on $\Omega = \mathbb{R}^3 \backslash B_R$, f obeys

$$-\Delta f = (\lambda_0^2 \sigma_0)^{-1} Ef$$

and so f vanishes on Ω by the argument preceding Theorem XIII.57. Thus, to conclude that f is zero we need a unique continuation theorem for H. But since $Hf = Ef$, we have that

$$(\Delta f)(x) = \alpha(x) f(x) + \beta(x) \cdot \nabla f(x)$$

for suitable bounded functions $\alpha(x)$ and $\beta(x)$, so that

$$|(\Delta f)(x)| \leq M(|f(x)| + |\nabla f(x)|)$$

By a slight extension of the methods of the Appendix (see Problem 113), there is a unique continuation theorem for such an inequality. ∎

Appendix to XIII.13 Unique continuation theorems for Schrödinger operators

In this appendix we shall prove Theorem XIII.57. In fact, we shall prove the following stronger theorem:

Theorem XIII.63 Let $u \in H^2_{\text{loc}}$, that is, $\varphi u \in D(-\Delta)$ for each $\varphi \in C_0^\infty(\mathbb{R}^n)$. Let D be an open connected set in $\mathbb{R}^n$ and suppose that

$$|\Delta u(x)| \leq M|u(x)|$$

almost everywhere in D. Then, if u vanishes in the neighborhood of a single point $x_0 \in D$, u is identically zero in D.

The proof of this result, which we give only when $n = 3$ (see Problems 111, 112 for general n), relies on the following beautiful estimate for a C^∞ function f with support in $\{x | 0 < |x| < R\}$:

$$\int |x|^\alpha |f(x)|^2 \, d^3x \leq \tfrac{4}{3}R^4 \int |x|^\alpha |\Delta f|^2 \, d^3x \tag{100}$$

for *all* real α. We shall prove (100) by using the "partial wave expansion" of f,

$$f(x) = \sum_{\ell, m} f_{\ell m}(|x|) Y_{\ell m}(\Omega_x)$$

described explicitly below. Thus, we begin by proving an analogue of (100) for each partial wave.

Lemma 1 Let f be a C^∞ function with support in $(0, 1)$. For each $\ell = 0, 1, 2, \ldots$, define

$$g_\ell = -f'' + \frac{\ell(\ell+1)}{x^2} f$$

Then for *any* real α

$$\int_0^1 x^\alpha |f(x)|^2 \, dx \leq \tfrac{4}{3}(2\ell+1)^{-2} \int_0^1 x^\alpha |g_\ell(x)|^2 \, dx$$

Proof Fix ℓ and let D denote the formal differential operator $-d^2/dx^2 + \ell(\ell+1)/x^2$. Then, as a formal operator, $Dh_+ = Dh_- = 0$ where $h_+(x) = x^{\ell+1}$ and $h_-(x) = x^{-\ell}$. Now, since f vanishes near zero and one, we can freely integrate by parts the expressions $\int f \, Dh_\pm = 0$ to conclude that

$$\int_0^1 g_\ell(x) h_\pm(x) \, dx = 0 \tag{101}$$

We claim that, setting $g = g_\ell$,

$$f(x) = [h_+(x)A(x) + h_-(x)B(x)]/(2\ell+1) \tag{102a}$$

$$A(x) = \int_x^1 g(y)h_-(y) \, dy; \qquad B(x) = \int_0^x g(y)h_+(y) \, dy \tag{102b}$$

(102) is a standard variation of parameters formula from ordinary differential equations which can be proven as follows: Let $F(x)$ denote the right-hand side of (102a). Then $DF = g$ since $h_+ h'_- - h'_+ h_- = 2\ell + 1$, and by (101) F has support strictly in (0, 1). Since $D(F - f) = 0$, and $F - f$ is zero near 0, $F - f = 0$ by the uniqueness of solutions of ordinary differential equations.

Next, we claim that for any β,

$$|A(x)x^\beta| \leq \int_0^1 |x^\beta h_-(x)g(x)|\ dx \tag{103a}$$

$$|B(x)x^\beta| \leq \int_0^1 |x^\beta h_+(x)g(x)|\ dx \tag{103b}$$

Suppose $\beta > 0$. Then,

$$|A(x)x^\beta| \leq x^\beta \int_x^1 y^{-\beta} |y^\beta h_-(y)g(y)|\ dy$$

$$\leq \int_x^1 y^\beta |h_-(y)g(y)|\ dy$$

If $\beta \leq 0$, we use (101) to rewrite A so that

$$|A(x)x^\beta| \leq x^\beta \int_0^x y^{-\beta} |y^\beta h_-(y)g(y)|\ dy$$

$$\leq \int_0^x |y^\beta h_-(y)g(y)|\ dy$$

This proves (103a); the proof of (103b) is similar.

As a result,

$$H(x) \equiv [x^{\alpha-2}|f(x)|^2]$$

$$\leq (2\ell + 1)^{-2}(|x^{\frac{1}{2}\alpha+\ell}A(x)| + |x^{\frac{1}{2}\alpha-\ell-1}B(x)|)^2$$

$$\leq \frac{4}{(2\ell + 1)^2}\left(\int_0^1 |x^{\alpha/2}g(x)|\ dx\right)^2$$

$$\leq \frac{4}{(2\ell + 1)^2}\int_0^1 x^\alpha |g(x)|^2\ dx$$

In particular

$$\int_0^1 x^\alpha |f(x)|^2\ dx = \int_0^1 x^2 H(x)\ dx \leq \frac{4}{3(2\ell + 1)^2}\int_0^1 x^\alpha |g(x)|^2\ dx \ \blacksquare$$

Lemma 2 Let h be in $C_0^\infty(\mathbb{R}^3)$ with support in $\{x \,|\, 0 < |x| < 1\}$. Then, for any real α,

$$\int |x|^\alpha |h(x)|^2 \, d^3x \leq \tfrac{4}{3} \int |x|^\alpha |\Delta h(x)|^2 \, d^3x$$

Proof We use the spherical harmonic decomposition described in Example 4 of the Appendix to Section X.1. There is a distinguished orthonormal basis $\{Y_{\ell m}(\Omega)\}$, $\ell = 0, 1, \ldots; m = -\ell, -\ell + 1, \ldots, \ell - 1, \ell$, of $L^2(S^2)$ where S^2 is the unit sphere in $\mathbb{R}^3$. Given $f \in L^2(\mathbb{R}^3)$, we define

$$f_{\ell,\, m}(r) = r \int f(r\Omega) \overline{Y_{\ell,\, m}(\Omega)} \, d\Omega$$

Then, for $f \in C_0^\infty$,

$$rf(r\Omega) = \sum_{\ell,\, m} f_{\ell m}(r) Y_{\ell m}(\Omega)$$

$$-r(\Delta f)(r\Omega) = \sum_{\ell,\, m} (D_\ell \, f_{\ell m})(r) Y_{\ell m}(\Omega)$$

where $D_\ell = -d^2/dr^2 + \ell(\ell + 1)r^{-2}$. Thus, using the orthonormality of the $Y_{\ell m}$, if h has support in $\{x \,|\, 0 < |x| < 1\}$,

$$\int |x|^\alpha |h(x)|^2 \, d^3x = \sum_{\ell,\, m} \int r^\alpha |h_{\ell m}(r)|^2 \, dr$$

$$\leq \sum_{\ell,\, m} \tfrac{4}{3}(2\ell + 1)^{-2} \int r^\alpha |D_\ell h_{\ell m}(r)|^2 \, dr$$

$$\leq \tfrac{4}{3} \int |x|^\alpha |\Delta h(x)|^2 \, d^3x$$

where we have used Lemma 1. ∎

Lemma 3 Suppose that $h \in L^2(\mathbb{R}^3, d^3x)$ lies in the domain of $-\Delta$ and that h vanishes outside some compact subset of $\{x \,|\, 0 < |x - a| < R\}$ for some $a \in \mathbb{R}^3$; $R > 0$. Then

$$\int |x - a|^\alpha |h(x)|^2 \, d^3x \leq \tfrac{4}{3} R^4 \int |x - a|^\alpha |\Delta h(x)|^2 \, d^3x \tag{104}$$

for *any* real α.

Proof Suppose first that $h \in C_0^\infty(\mathbb{R}^3)$. Then (104) follows from Lemma 2 after the change of variables $y = (x - a)/R$. Knowing (104) for all $h \in C_0^\infty(\mathbb{R}^3)$ with the required support property yields (104) for all $h \in D(-\Delta)$ by a simple approximate identity argument. ∎

Proof of Theorem XIII.63 For each $x \in D$, define

$$R_x = \min\{(\tfrac{128}{3} M^2)^{-1/4}, \tfrac{1}{2} \operatorname{dist}(x, \partial D)\}$$

We claim that, if $u(x)$ vanishes for x near y and obeys $|\Delta u(x)| \leq M|u(x)|$, then $u(x)$ vanishes in $\{x \,|\, |x-y| \leq R_y\}$. Accepting this claim for the moment, let us prove that $u \equiv 0$ if u vanishes near some $x_0 \in D$. Given $y \in D$, choose a smooth curve γ in D joining x_0 to y. Suppose that γ has length L. Since γ is compact, $\operatorname{dist}(x, \partial D)$ is bounded away from zero on γ so R_x is bounded below on γ, say by R_0. Choose an integer n so that $\frac{1}{2}R_0 n \geq L > \frac{1}{2}R_0(n-1)$, and $x_1, \ldots, x_{n-1}, x_n = y$ on γ so that the length of γ between x_i and x_{i-1} $(i = 1, \ldots, n-1)$ is $\leq \frac{1}{2}R_0$. In particular, $|x_i - x_{i-1}| \leq \frac{1}{2}R_0$. Since u vanishes near x_0, by our claim, it vanishes if $|x - x_0| < R_0$ and so near x_1. Repeating this argument, we see that $u(y) = 0$, so $u \equiv 0$ in D.

We now turn to the proof of the claim. Fix y and let χ be a function in C_0^∞ that is 1 if $|x-y| \leq R_y$ and 0 if $|x-y| \geq \frac{3}{2}R_y$. Then χu has support in $\{x \,|\, 0 < |x-y| < 2R_y\}$ so, by Lemma 3, for any $\beta > 0$,

$$\int_{|x-y|\leq R_y} |x-y|^{-\beta}|u(x)|^2\,dx$$

$$\leq \int |x-y|^{-\beta}|(\chi u)(x)|^2\,dx$$

$$\leq \tfrac{4}{3}(2R_y)^4 \int_{|x-y|\leq 2R_y} |x-y|^{-\beta}|\Delta(\chi u)(x)|^2\,dx$$

$$\leq \tfrac{64}{3}M^2R_y^4 \int_{|x-y|\leq R_y} |x-y|^{-\beta}|u(x)|^2\,dx + CR_y^{-\beta}$$

$$\leq \tfrac{1}{2}\int_{|x-y|\leq R_y} |x-y|^{-\beta}|u(x)|^2\,dy + CR_y^{-\beta}$$

where

$$C = \tfrac{64}{3}R_y^4 \int_{R_y\leq|x-y|\leq 2R_y} |\Delta(\chi u)|^2\,dx$$

is finite since $\chi u \in D(-\Delta)$. Therefore, if $R_1 < R_y$,

$$\int_{|x-y|\leq R_1} |u(x)|^2\,dx \leq R_1^\beta \int_{|x-y|<R_y} |x-y|^{-\beta}|u(x)|^2\,dx$$

$$\leq 2C(R_1/R_y)^\beta$$

Letting β go to infinity, we see that $\int_{|x-y|\leq R_1} |u(x)|^2\,dx = 0$. This proves our claim, and thus the result. ∎

We are now ready to restate and prove Theorem XIII.57.

Theorem XIII.57 Let V be a function on $\mathbb{R}^n$ so that:

(i) Multiplication by V is $-\Delta$-bounded with relative bound less than 1.
(ii) There is a closed set S of measure zero so that $\mathbb{R}^n \backslash S$ is connected and so that V is bounded on any compact subset of $\mathbb{R}^n \backslash S$.

Let $H = -\Delta + V$ and suppose that $Hu = Eu$ for some E and $u \in L^2$. Suppose that u vanishes on an open subset of $\mathbb{R}^n$. Then u is identically zero.

Proof Suppose that u vanishes near $x_0 \in \mathbb{R}^n \backslash S$. By choosing a neighborhood of a curve between x_0 and some $y \in \mathbb{R}^n \backslash S$ we can find an open connected set $D \subset \mathbb{R}^n \backslash S$, with $x_0, y \in D$, so that $\bar{D}$ is compact in $\mathbb{R}^n \backslash S$. Since V is bounded on D, say by M_0, and $u \in D(-\Delta + V) = D(-\Delta)$,

$$|-\Delta u| \leq (M_0 + |E|)|u|$$

on D, so u vanishes in D by Theorem XIII.63. It follows that u is zero on $\mathbb{R}^n \backslash S$. ∎

XIII.14 Compactness criteria and operators with compact resolvent

In most of this chapter we have studied the continuous spectrum of self-adjoint operators, especially Schrödinger operators with potentials that decay at infinity. In this section, by contrast, we concentrate on criteria for proving that an operator has purely discrete spectrum. First, we show that a semibounded self-adjoint operator A has entirely discrete spectrum if and only if its resolvent is a compact operator. To apply this result, we need criteria that guarantee that certain subsets of L^2 are compact; these criteria are supplied by results of Rellich and Riesz. We then apply these techniques to provide extensions of Theorem XIII.16 which shows that Schrödinger operators with potentials that grow at infinity have purely discrete spectrum.

These ideas are intimately connected with various compact embedding theorems for Sobolev spaces which are required in various applications to partial differential equations and, in particular, in the Lax–Phillips theory (Section XI.11). In the middle part of this section we describe these embedding theorems.

As a further application, we show that the Hamiltonian H associated to a statistical mechanical system in a box has purely discrete spectrum and that $e^{-\beta H}$ is trace class. We conclude the section by giving criteria that guarantee that part of the spectrum of a self-adjoint operator is discrete.

Theorem XIII.64 Let A be a self-adjoint operator that is bounded from below. Then the following are equivalent:

(i) $(A-\mu)^{-1}$ is compact for some $\mu \in \rho(A)$.
(ii) $(A-\mu)^{-1}$ is compact for all $\mu \in \rho(A)$.
(iii) $\{\psi \in D(A) \mid \|\psi\| \leq 1;\ \|A\psi\| \leq b\}$ is compact for all b.
(iv) $\{\psi \in Q(A) \mid \|\psi\| \leq 1,\ (\psi, A\psi) \leq b\}$ is compact for all b.
(v) There exists a complete orthonormal basis $\{\varphi_n\}_{n=1}^{\infty}$ in $D(A)$ so that $A\varphi_n = \mu_n \varphi_n$ with $\mu_1 \leq \mu_2 \leq \cdots$ and $\mu_n \to \infty$.
(vi) $\mu_n(A) \to \infty$ where $\mu_n(\cdot)$ is given by the min–max principle.

Proof We shall prove (i)$\Leftrightarrow$(ii); (v)$\Leftrightarrow$(vi); (v)$\Rightarrow$(iv)$\Rightarrow$(iii)$\Rightarrow$(i)$\Rightarrow$(v).

(i)$\Leftrightarrow$(ii) is trivial in one direction and follows in the other by the first resolvent formula and the fact that the compact operators are an ideal.

(v)$\Leftrightarrow$(vi) follows directly from the min–max principle, Theorem XIII.1.

(v)$\Rightarrow$(iv) Let

$$F_b = \{\psi \in Q(A) \mid \|\psi\| \leq 1,\ (\psi, A\psi) \leq b\}$$

We will prove that F_b is closed and that, for any ε, it can be covered by finitely many open balls of radius ε. It easily follows from this that it is compact (Problem 114). Let $\psi_n \in F_b$ with $\psi_n \to \psi$. Then clearly $\|\psi\| \leq 1$, so we need only show that $\psi \in Q(A)$ and $(\psi, A\psi) \leq b$. It is clearly sufficient to prove that for any $\lambda < \infty$, $(\psi, AP_{(-\infty,\lambda)}\psi) \leq b$ where P_Ω is the family of spectral projections for A. But, since $AP_{(-\infty,\lambda)}$ is bounded,

$$\begin{aligned}(\psi, AP_{(-\infty,\lambda)}\psi) &= \lim_{n\to\infty} (\psi_n, AP_{(-\infty,\lambda)}\psi_n) \\ &\leq \lim_{n\to\infty} (\psi_n, A\psi_n) \leq b\end{aligned}$$

Thus F_b is closed. Now let $-a$ be a lower bound for A so that $B = A + a \geq 0$ and $\psi \in F_b$ implies $(\psi, B\psi) \leq b + a$. Given ε, choose N so that $\mu_N + a \geq 2\varepsilon^{-1}(b+a)$. Then $(\psi, B\psi) \leq b + a$ and hypothesis (v) imply that

$$\sum_{n \geq N} |(\psi, \varphi_n)|^2 \leq \tfrac{1}{2}\varepsilon$$

Thus any $\psi \in F_b$ is within $\sqrt{\varepsilon/2}$ of a point of the unit ball in the subspace generated by $\{\varphi_1, \ldots, \varphi_{N-1}\}$. Since this ball can be covered by finitely many $\sqrt{\varepsilon}/2$-balls, F_b can be covered by finitely many ε-balls.

(iv)$\Rightarrow$(iii) The set

$$D_b = \{\psi \in D(A) \mid \|\psi\| \leq 1,\ \|A\psi\| \leq b\}$$

is closed by an argument similar to that proving F_b closed. By the Schwarz inequality, $D_b \subset F_b$, so D_b is compact if F_b is compact.

$(iii) \Rightarrow (i)$ Without loss of generality, we may assume that A is positive. Let $M = \{\psi = (A+1)^{-1}\varphi \mid \|\varphi\| \leq 1\}$. Suppose that $\psi \in M$ and $\varphi = (A+1)\psi$. Then

$$\|\psi\| \leq \|(A+1)^{-1}\| \, \|\varphi\| \leq \|\varphi\| \leq 1$$

and

$$\|A\psi\| \leq \|A(A+1)^{-1}\| \, \|\varphi\| \leq \|\varphi\| \leq 1$$

so $\psi \in D_1$. Thus, $\bar{M} \subset \bar{D}_1$ so that D_1 being compact implies that M is pre-compact, i.e., that $(A+1)^{-1}$ is a compact operator.

$(i) \Rightarrow (v)$ Since (i) $\Rightarrow$ (ii), we may suppose that $(A+a)^{-1}$ is compact where a is real and $-a$ is a strict lower bound for A. Since $(A+a)^{-1}$ is compact, the Hilbert–Schmidt theorem (Theorem VI.16) assures us that there exists an orthonormal basis $\{\varphi_n\}$ with $(A+a)^{-1}\varphi_n = \lambda_n \varphi_n$ and $\lambda_n \to 0$. Since $(A+a)^{-1}$ is positive, $\lambda_n \geq 0$, so we can renumber the λ's and φ's to ensure that $\lambda_1 \geq \lambda_2 \geq \cdots$. Taking $\mu_n = \lambda_n^{-1} - a$, (v) follows. ∎

On account of the criteria (iii), (iv) of Theorem XIII.64, it is important to have criteria that assure us that a subset S of $L^2(\mathbb{R}^n)$ is compact. To see the ideas involved, consider first the case where $\mathscr{H} = L^2(-\pi, \pi)$ and A is the self-adjoint extension of $i\, d/dx \restriction C_0^\infty(-\pi, \pi)$ with boundary conditions $\varphi(-\pi) = \varphi(\pi)$. Let

$$S = \{\psi \in L^2(-\pi, \pi) \mid \|\psi\| \leq 1, \, \|A\psi\| \leq 1\}$$

Expanding each $\psi \in S$ in its Fourier series, we can map S isometrically onto

$$\hat{S} = \{\{a_n\} \in \ell_2(-\infty, \infty) \mid \sum |a_n|^2 \leq 1, \sum n^2 |a_n|^2 \leq 1\}$$

The second condition ensures that the tails of sequences in $\hat{S}$ are uniformly small and using this it is easy to show that $\hat{S}$ is compact (Problem 115), which proves that S is compact. This situation is reminiscent of Ascoli's theorem where compactness of support, uniform boundedness, and uniform equicontinuity combined to guarantee compactness of a set of functions. In this case the uniform equicontinuity is replaced by the smoothness condition, $\|A\psi\| \leq 1$ for all $\psi \in S$, which is equivalent to a decay condition on the Fourier coefficients of ψ. If we now try to extend this idea to $L^2(\mathbb{R})$, it is clear that the smoothness condition itself is not enough. For given any $f \in C_0^\infty(-\pi, \pi)$, the set of translates $f_n(x) = f(x + 2n\pi)$ cannot have any convergent subsequence. The difficulty is that these functions are not uniformly small for large x. So this suggests that to get a compact set in $L^2(\mathbb{R})$ we should require both the functions and their Fourier transforms to be "uniformly small" at ∞. This is just the hypothesis of Rellich's criterion below.

We give a short proof of Rellich's criterion based on Weyl's theorem and Theorem XIII.64. A longer proof which follows the Fourier series intuition we have just discussed is outlined in Problem 116.

Definition Let F be a function on $\mathbb{R}^n$ that is measurable and nonnegative almost everywhere. We say that $F \to \infty$ if and only if, for every $N > 0$, there is an R_N so that $F(x) \geq N$ for almost all x with $|x| \geq R_N$.

Theorem XIII.65 (Rellich's criterion) Let F and G be two functions on $\mathbb{R}^n$ so that $F \to \infty$ and $G \to \infty$. Then

$$S = \left\{ \psi \;\middle|\; \int |\psi(x)|^2 \, dx \leq 1, \int F(x)|\psi(x)|^2 \, dx \leq 1, \int G(p)|\hat{\psi}(p)|^2 \, dp \leq 1 \right\}$$

is a compact subset of $L^2(\mathbb{R}^n)$.

Proof We use the basic idea behind the proof of Theorem XIII.16. By replacing F by $\min\{F(x), x^2\}$ and similarly changing G, we can suppose without loss that $F(x) \leq x^2$ and $G(p) \leq p^2$. Thus we can define a self-adjoint operator $A = G(p) + F(x)$ as a densely defined form sum on $Q(G(p)) \cap Q(F(x))$. By the proof in Theorem XIII.64, S is closed. Further, since

$$S \subset \{\psi \in L^2 \mid \|\psi\| \leq 1, (\psi, A\psi) \leq 2\}$$

it suffices to show that $\mu_m(A) \to \infty$ as $m \to \infty$ by the equivalence (iv) $\Leftrightarrow$ (vi) in Theorem XIII.64.

Now let V be a bounded function of compact support. Then, we claim that $V(x)(G(p) + 1)^{-1}$ is compact: For $V(x)(\varepsilon p^n + G(p) + 1)^{-1}$ is Hilbert–Schmidt since $(\varepsilon p^n + G(p) + 1)^{-1}$ is in L^2. Moreover, since $G \to \infty$, $(\varepsilon p^n + G(p) + 1)^{-1} \to (G(p) + 1)^{-1}$ in L^∞ as $\varepsilon \downarrow 0$, so $V(x)(G(p) + 1)^{-1}$ is a norm limit of Hilbert–Schmidt operators.

From Weyl's theorem (Theorem XIII.14), we see that $G(p) + V(x)$ has discrete spectrum in $(-\infty, 0)$ so that, in particular, $\mu_m(G(p) + V(x)) \geq -1$ for m sufficiently large.

Given $\alpha > 0$, define V_α by

$$V_\alpha(x) = \min\{F(x), \alpha + 1\} - \alpha - 1$$

V_α has compact support since $F \to \infty$. Since

$$\mu_m(A) \geq \mu_m(G(p) + V_\alpha(x)) + \alpha + 1$$

we see that $\mu_m(A) \geq \alpha$ for m sufficiently large. Since α is arbitrary, $\mu_m(A) \to \infty$ as $m \to \infty$. ∎

Theorem XIII.66 (M. Riesz's criterion) Let $p < \infty$. Let $S \subset L^p(\mathbb{R}^n)_1$, the unit ball in L^p. A necessary and sufficient condition that the norm closure of S be norm compact is that:

(1) $f \to 0$ in L^p sense at infinity uniformly in S, i.e., for any ε, there is a bounded set $K \subset \mathbb{R}^n$ so that

$$\int_{\mathbb{R}^n \setminus K} |f(x)|^p \, dx \leq \varepsilon^p \tag{105}$$

for all $f \in S$;

and

(2) $f(\cdot - y) \to f$ uniformly in S as $y \to 0$, i.e., for any ε, there is a δ so that $f \in S$ and $|y| < \delta$ imply that

$$\int_{\mathbb{R}^n} |f(x - y) - f(x)|^p \, dx \leq \varepsilon^p \tag{106}$$

Proof Suppose first that $\bar{S}$ is compact. Fix $\alpha > 0$. Find $f_1, \ldots, f_n$ so that the $(\alpha/3)$-balls about the f_i cover S. Then find K and δ so that (105) and (106) hold for $f = f_1, \ldots, f_n$ and $\varepsilon = \alpha/3$. This can be done since for any $g \in L^p$, $\lim_{K \uparrow \mathbb{R}^n} \int_{\mathbb{R}^n \setminus K} |g|^p \, dx = 0$ and $g(\cdot - y) \to g$. By an $\alpha/3$ argument, (105) and (106) hold with $\varepsilon = \alpha$.

Conversely, suppose that S obeys (1) and (2). For any compact $\Omega \subset \mathbb{R}^n$ and finite numbers α, β,

$$T(\Omega, \alpha, \beta) = \{f \in C_0^\infty(\mathbb{R}^n) \mid \operatorname{supp} f \subset \Omega, \|f\|_\infty \leq \alpha, \|\nabla f\|_\infty \leq \beta\}$$

is precompact in $C(\Omega)$ by Ascoli's theorem, and so a fortiori precompact in $L^p(\mathbb{R}^n)$. Thus, it suffices, given ε, to find Ω, α and β so that given $f \in S$, there is a $g \in T(\Omega, \alpha, \beta)$ with $\|f - g\|_p < \varepsilon$. For since T can be covered by finitely many ε-balls, we can conclude that S can be covered by finitely many 2ε-balls.

Given ε, find K and δ so that for $f \in S$ and $|y| \leq \delta$:

$$\int_{\mathbb{R}^n \setminus K} |f(x)|^p \, dx \leq (\varepsilon/4)^p$$

$$\|f(\cdot - y) - f\|_p \leq \varepsilon/4$$

Let η be any C^∞ function supported in $\{y \mid |y| < \delta\}$ with $\int \eta(x) \, dx = 1$ and let χ be the characteristic function of $K' = \{y \mid \operatorname{dist}(y, K) < \delta\}$. Let $\Omega = \{y \mid \operatorname{dist}(y, K) \leq 2\delta\}$, $\alpha = \|\eta\|_q$, and $\beta = \|\nabla\eta\|_q$, where $q = p(p-1)^{-1}$. Given $f \in S$, let $g = \eta * (\chi f)$. We claim that

$$\|g - f\|_p \leq \varepsilon \tag{107}$$

Moreover, $g \in T(\Omega, \alpha, \beta)$, for it is evident that supp $g \subset \Omega$ and the norm conditions follow from Young's inequality.

Thus, we need only prove (107) to see that $\bar{S}$ is compact. Now, by choice of K and the definition of K', if $|y| < \delta$,

$$\int_{\mathbb{R}^n \setminus K'} |f(x-y)|^p \, dx \leq \int_{\mathbb{R}^n \setminus K} |f(x)|^p \, dx \leq (\varepsilon/4)^p$$

so

$$\begin{aligned} \|(\chi f)(\cdot - y) - \chi f\|_p &\leq \|f(\cdot - y) - f\|_p + \|(1-\chi)f\|_p \\ &\quad + \|[1 - \chi(\cdot - y)]f(\cdot - y)\|_p \\ &\leq 3\varepsilon/4 \end{aligned}$$

Thus,

$$\|\eta * \chi f - \chi f\|_p \leq \int \eta(y) \|\chi f(\cdot - y) - \chi f\|_p \, dy \leq 3\varepsilon/4$$

so

$$\|g - f\|_p \leq \|g - \chi f\|_p + \|(1-\chi)f\|_p \leq \varepsilon \quad \blacksquare$$

Using these last two theorems, we can completely analyze the spectrum of Schrödinger operators with potentials going to infinity at infinity. The following result strengthens Theorem XIII.16.

Theorem XIII.67 Let $V \in L^1_{\text{loc}}(\mathbb{R}^n)$ be bounded from below and suppose that $V \to \infty$. Then $H = -\Delta + V$ defined as a sum of quadratic forms is an operator with compact resolvent. In particular, H has purely discrete spectrum and a complete set of eigenfunctions.

Proof By Theorem XIII.64, we need only show that

$$F_H \equiv \{\psi \in Q(H) \mid \|\psi\| \leq 1, (\psi, H\psi) \leq b\}$$

is compact. Since it is closed by the arguments of Theorem XIII.64, we need only prove it is contained in a compact set. But, since $-\Delta$ and V are positive definite, $(\psi, H\psi) \leq b$ implies that $(\psi, -\Delta\psi) \leq b$ and $(\psi, V\psi) \leq b$ so

$$F_H \subset \left\{ \psi \;\middle|\; \|\psi\| \leq 1, \int p^2 |\hat{\psi}(p)|^2 \, dp \leq b, \int V(x)|\psi(x)|^2 \, dx \leq b \right\}$$

and this set is compact by Rellich's criterion. $\blacksquare$

To extend this last result to the case where V has some negative singularities, we first prove a simple perturbation result.

Theorem XIII.68 Let A be a semibounded self-adjoint operator with compact resolvent. Let b be a symmetric form-bounded perturbation of A with relative form bound strictly smaller than 1. Let $C = A + b$ defined as a sum of forms. Then C has compact resolvent.

Proof By hypothesis,

$$|b(\psi, \psi)| \leq \alpha(\psi, A\psi) + \beta(\psi, \psi)$$

with $\alpha < 1$. Then for any $\psi \in Q(C) = Q(A)$,

$$(\psi, C\psi) \geq (1 - \alpha)(\psi, A\psi) - \beta(\psi, \psi)$$

It follows from the form version of the min–max principle (Theorem XIII.2) that

$$\mu_n(C) \geq (1 - \alpha)\mu_n(A) - \beta$$

Since $\mu_n(A) \to \infty$, we conclude that $\mu_n(C) \to \infty$, so C has a compact resolvent by criterion (vi) of Theorem XIII.64. ∎

Theorem XIII.69 Let $n \geq 3$. Let $V = V_1 + V_2$ where $V_2 \in L^{n/2}(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$, $V_1 > 0$, $V_1 \to \infty$, and $V_1 \in L^1_{\text{loc}}(\mathbb{R}^n)$. Then $H = -\Delta + V_1 + V_2$, defined as a sum of quadratic forms, is an operator with compact resolvent.

Proof By a form version of Strichartz theorem (Problem 119), V_2 is $-\Delta$-form bounded with relative bound zero. So, since V_1 is positive, V_2 is also $(-\Delta + V_1)$-form bounded with relative bound zero. The result now follows from Theorems XIII.67 and XIII.68. ∎

As a result of the above considerations, we have a complete qualitative description of the spectrum of $-\Delta + V$ when $V \to \infty$. What more can we ask for in a general framework? The actual eigenvalues $\lambda_n(V) \equiv \mu_n(-\Delta + V)$, and corresponding eigenfunctions $\psi_n(x)$, are obviously dependent on detailed information about V and change as V changes locally, but one can hope that the qualitative behavior of $\lambda_n(V)$ as $n \to \infty$ and $\psi_n(x)$ as $x \to \infty$ depends only on the qualitative behavior of V as $x \to \infty$. For the case of eigenvalues, we shall study this problem in Section 15, but we can use the methods of Section 11 to study the behavior of $\psi_n(x)$ as $x \to \infty$.

Theorem XIII.70 Suppose that H obeys the hypotheses of Theorem XIII.69. Then any eigenfunction of H obeys $\psi(x) \in D(e^{a|x|})$ for any $a > 0$. If $V \geq 0$, then for any $a > 0$, there is a C with

$$|\psi(x)| \leq Ce^{-a|x|}$$

Proof As in the proof of Theorem XIII.39, we need only prove that ψ is an entire vector for $W(\alpha) = e^{i\alpha x_j}$ for each j to conclude that $\psi \in D(\exp(a|x|))$ for all $a > 0$. As in that theorem

$$W(\alpha)HW(\alpha)^{-1} = -\sum_{i \neq j} \partial_i^2 + (i\,\partial_j + \alpha)^2 + V \tag{108}$$

for α real. The right-hand side of (108) defines an entire analytic family of type (B) (see Section XII.2) for all complex α. Since $(H(\alpha) - \lambda)^{-1}$ is compact for α real, it is compact for all α. Moreover, as in the proof of the Theorem XIII.39, $H(\alpha)$ has locally constant spectrum. Using the compactness of the resolvent it is easy to see that $H(\alpha)$ has spectrum independent of α (Problem 121), so by O'Connor's lemma, all its eigenfunctions are entire in α. This proves the first assertion.

Now suppose that V is positive. Fix k and for $a \in \mathbb{R}$, let

$$H_0(a) = (i\,\partial_k - ia)^2 - \sum_{j \neq k} \partial_j^2 = e^{ax_k} H_0\, e^{-ax_k}$$

Then $\exp(-tH_0(a))$ has the kernel

$$(4\pi t)^{-n/2} e^{ax_k} e^{-|x-y|^2/4t} e^{-ay_k}$$

and so is positivity preserving. Moreover, since this kernel is an L^2 function of $x - y$, Young's inequality implies that for any $t > 0$,

$$\|e^{-tH_0(a)}\psi\|_\infty \leq C_{a,t} \|\psi\|_2 \tag{109}$$

Now, let V_n be a monotone increasing sequence of bounded multiplication operators with $V_n \uparrow V$. Then $H_0(a) + V_n$ converges to $H_0(a) + V$ in strong resolvent sense (by a monotone convergence theorem for forms) so

$$e^{-t(H_0(a)+V)} = \operatorname*{s-lim}_{n\to\infty} \operatorname*{s-lim}_{m\to\infty} [e^{-tH_0(a)/m} e^{-tV_n/m}]^m$$

Since $e^{-tH_0(a)/m}$ is positivity preserving and $0 \leq e^{-tV_n/m} \leq 1$, we conclude that

$$|e^{-t(H_0(a)+V)} f| \leq e^{-tH_0(a)} |f|$$

pointwise a.e. But by (109), $\exp(-tH_0(a))|f| \in L^\infty$. Thus for any $f \in L^2$, $e^{-t(H_0(a)+V)} f \in L^\infty$; and, in particular, eigenfunctions of $H_0(a) + V$ are in L^∞. But, if ψ is an eigenfunction of $H_0 + V$, then $H_0(a) + V$ has $e^{ax_k}\psi$ as an eigenfunction. Thus $e^{ax_k}\psi \in L^\infty$ for all a, which proves the second result. ∎

The eigenfunctions of $-\Delta + x^2$ are Gaussians times products of Hermite polynomials, so the previous result on falloff faster than any exponential is far from optimal. One expects stronger results to hold if V goes to infinity fast enough. First, one can simply generalize the Combes–Thomas method a little further:

Theorem XIII.71 Let V have form of Theorem XIII.69. Let $W(x) = \int_0^{|x|} \sqrt{V_0(s)}\, ds$ where $V_0(r) = \text{ess inf}_{|x|=r} V_1(x)$. Then for any eigenfunction ψ of $-\Delta + V$, $\psi \in D(\exp(\frac{1}{2}\beta W(x)))$ for any $\beta < \sqrt{5} - 1$.

Proof Let $U(\alpha) = \exp(i\alpha W(x))$. Then,

$$U(\alpha)(-\Delta)U(\alpha)^{-1} = (i\nabla + \alpha\nabla W)^2$$

$$= -\Delta + \alpha^2(\nabla W)^2 + \alpha(\nabla W)\cdot(i\nabla) + \alpha(i\nabla)\cdot(\nabla W)$$

But $|\nabla W| = V_0^{1/2} \leq V_1^{1/2}$, so

$$\alpha^2(\nabla W)^2 \leq \alpha^2(-\Delta + V_2 + C) + \alpha^2(\nabla W)^2 \leq \alpha^2(-\Delta + V + \text{const})$$

and

$$\pm[\alpha(\nabla W)\cdot(i\nabla) + \alpha(i\nabla)\cdot\nabla W] \leq (|\alpha| + \varepsilon)(-\Delta + V + \text{const})$$

so $U(\alpha)(-\Delta + V)U(\alpha)^{-1}$ extends to an analytic family in the region $|\alpha|^2 + |\alpha| < 1$. The result now follows by mimicking the method of proof of the last theorem. ∎

By totally different methods, one can prove the following sharper result (see the references in the Notes for a proof):

Theorem XIII.72 Let V be a positive C^∞ function on $\mathbb{R}^n$ and let $H = -\Delta + V$. Suppose that ψ is an eigenfunction for H. Then:

(a) If $V(x) \geq c|x|^{2n} - d$ for some c and d, then for every $\varepsilon > 0$, there is a D with

$$|\psi(x)| \leq D \exp(-(n+1)^{-1}(c-\varepsilon)^{1/2}|x|^{n+1})$$

for all x.

(b) If $V(x) \leq c|x|^{2n} + d$ for some c and d and ψ is the ground state wave function then, for any $\varepsilon > 0$, there is an $E > 0$ with

$$\psi(x) \geq E \exp(-(n+1)^{-1}(c+\varepsilon)^{1/2}|x|^{n+1})$$

The results of these preceding two theorems can be understood in terms of the WKB approximation,

$$\psi \sim \exp\left(-\int \sqrt{V-E}\, dx\right)$$

* * *

We turn now to compact embedding theorems for local Sobolev spaces. There are at least two natural candidates:

Definition Let $\Lambda \subset \mathbb{R}^n$ be an open set. $H^m(\Lambda)$ is the set of functions $f \in L^2(\Lambda)$ whose distributional derivatives $D^\alpha f$ are in $L^2(\Lambda)$ for all α with $|\alpha| \leq m$. $H^m(\Lambda)$ is a Hilbert space under the norm

$$\|f\|_m = \left(\sum_{|\alpha|\leq m} \|D^\alpha f\|_2^2\right)^{1/2}$$

$H_0^m(\Lambda)$ is defined to be the completion of $C_0^\infty(\Lambda)$ in the norm $\|\cdot\|_m$. $H^m(\Lambda)$ and $H_0^m(\Lambda)$ are called **local Sobolev spaces.**

In general, $H_0^m(\Lambda)$ is a proper subset of $H^m(\Lambda)$.

Example 1 Let $\Lambda = (0, 1) \subset \mathbb{R}$. Let $g(x) = e^x$ and let $f \in C_0^\infty(\Lambda)$. In the natural inner product on $H^1(\Lambda)$,

$$(g, f)_1 = \left(\left(-\frac{d}{dx^2} + 1\right)g, f\right)_{L^2} = 0$$

Thus $H_0^1(\Lambda) \subset \{g\}^\perp$ so that $H_0^1(\Lambda) \neq H^1(\Lambda)$.

The reader familiar with the theory of self-adjoint extensions (Section X.1) will notice a connection between Example 1 and the fact that $-d^2/dx^2$ is not essentially self-adjoint on $C_0^\infty(0, 1)$. In fact, using the fact that $-\Delta$ is never essentially self-adjoint on $C_0^\infty(\Lambda)$ for *bounded* Λ, one can show that $H_0^1(\Lambda)$ is always different from $H^1(\Lambda)$ for *bounded* Λ. Notice that $H_0^m(\mathbb{R}^n) = H^m(\mathbb{R}^n) = D((-\Delta)^{m/2})$.

There are many embedding relations for these Sobolev spaces.

Proposition Let Λ and Λ' be open sets with $\Lambda \subset \Lambda'$ and suppose that $m \geq j \geq 0$. Then:

(a) $H_0^m(\Lambda) \subset H^m(\Lambda)$.
(b) $H^m(\Lambda) \subset H^j(\Lambda)$.

(c) $H_0^m(\Lambda) \subset H_0^j(\Lambda)$.
(d) Let $f \in H(\Lambda')$. Then $f \restriction \Lambda$, the restriction of f to Λ, lies in $H^m(\Lambda)$.
(e) If $f \in H^m(\Lambda)$ and $f = 0$ on $\Lambda \backslash C$ where C is a compact subset of Λ, then $f \in H_0^m(\Lambda)$.
(f) If f is in $D((-\Delta)^{m/2})$ where $-\Delta$ denotes the operator on $L^2(\mathbb{R}^n)$, then $f \restriction \Lambda \in H^m(\Lambda)$.

All inclusions are norm nonincreasing.

Proof (a), (b), and (d) follow immediately from the definitions. (c) comes by using the norm inequality implicit in (b) and taking completions of $C_0^\infty(\mathbb{R}^n)$. (e) is an elementary "approximation of the identity" argument, and (f) follows by using the Fourier transform to estimate each term in $\|f\|_{H^m(\mathbb{R}^n)}$ in terms of $\|(-\Delta)^{m/2} f\|_{L^2}$ and $\|f\|_{L^2}$. ∎

We now prove two easy compactness results.

Theorem XIII.73 Let A be the Friedrichs extension of $-\Delta$ on $C_0^\infty(\Lambda)$ (the Dirichlet Laplacian). Suppose that Ω is bounded. Then:
(a) $H_0^m(\Lambda) \subset D(A^{m/2})$ and the norms are equivalent.
(b) If $m > j$, then the unit ball of $H_0^m(\Lambda)$ is a compact subset of $H_0^j(\Lambda)$.

Proof Let $f \in C_0^\infty(\Lambda)$. Then $\|f\|_m$ and $\|(-\Delta)^{m/2} f\|$ are equivalent norms since we can think of f as an element of L^2 in which case the derivatives of f obey $\mathscr{F}(D^\alpha f) = (ik)^\alpha \hat{f}$ and

$$k^{2m} \leq C_1 \sum_{|\alpha| \leq m} (k^\alpha)^2 \leq C_2(k^{2m} + 1)$$

Now clearly $C_0^\infty(\Lambda) \subset D(A^n)$ for all n and $A^n f = (-\Delta)^n f$, so that

$$\|\Delta^{m/2} f\|^2 = (f, (-\Delta)^m f) = (f, A^m f) = \|A^{m/2} f\|^2$$

As a result, the completion of C_0^∞ in the $\|\cdot\|_m$ norm is clearly in $D(A^{m/2})$.

Next, we claim that A is an operator with compact resolvent. To show that $F_b \equiv \{\psi \in Q(A) \mid \|\psi\| \leq 1, (\psi, A\psi) \leq b\}$ is compact in $L^2(\Lambda)$, it clearly suffices to prove that it is contained in a compact subset of $L^2(\mathbb{R}^n)$. But, as above $Q(A) \subset Q(-\Delta)$ with $(\psi, A\psi) = (\psi, -\Delta\psi)$ where $-\Delta$ means the usual operator on $L^2(\mathbb{R}^n)$. Let F be any function that is 1 on Λ with $F \to \infty$. Then

$$F_b \subset \{\psi \in L^2(\mathbb{R}^n) \mid \|\psi\| \leq 1, (\psi, -\Delta\psi) \leq b, (\psi, F\psi) \leq 1\}$$

so by Theorem XIII.65, F_b is contained in a compact subset of $L^2(\mathbb{R}^n)$.

Since $(A+1)^{-1}$ is compact from $L^2(\Lambda)$ to $L^2(\Lambda)$, it is compact from $D(A^{m/2})$ to $D(A^{m/2})$ for any m because the unitary map $(A+1)^{-m/2}$ from $L^2(\Lambda)$ to $D(A^{m/2})$ commutes with $(A+1)^{-1}$. Since $(A+1)^{-1}$ is compact, so is $(A+1)^{-1/2}$; thus, the unit ball of $D(A^{(m+1)/2})$ is compact in $D(A^{m/2})$. Since $H_0^j(\Lambda)$ is a subset of $D(A^{j/2})$, the compactness result on the H_0^j follows. ∎

We warn the reader that although $H_0^1(\Lambda) = D(A^{1/2})$ by the definition of A, $H_0^m(\Lambda)$ are unequal to $D(A^{m/2})$ for $m > 1$.

Corollary Let Ω be a bounded open set in $\mathbb{R}^n$. The Dirichlet Laplacian $-\Delta_D^\Omega$ has compact resolvent.

Proof By Theorem XIII.73,

$$\{\psi \in Q(-\Delta_D^\Omega) \mid (\psi, -\Delta_D^\Omega \psi) \leq 1 \text{ and } \|\psi\| \leq 1\}$$

is compact in $L^2(\Omega)$, so by Theorem XIII.64, $-\Delta_D^\Omega$ has compact resolvent. ∎

Lemma Let Λ be a bounded open set and let Λ' be open with $\bar{\Lambda} \subset \Lambda'$. Then there exists $\eta \in C_0^\infty(\Lambda')$ with $\eta \equiv 1$ on Λ.

Proof For any $x \in \bar{\Lambda}$, find an $r_x > 0$ so that the ball of radius $2r_x$ about x lies in Λ'. By compactness, we can cover $\bar{\Lambda}$ by a finite number of balls $B_1, \ldots, B_m$ with radii r_{x_i}. In the usual way find $\eta_i \in C_0^\infty(\mathbb{R}^n)$ with $\eta_i \equiv 1$ on B_i and $\operatorname{supp} \eta_i$ in the ball of radius $2r_{x_i}$ about x_i. Now, just define $\eta = 1 - \prod_{i=1}^m (1 - \eta_i)$. ∎

Theorem XIII.74 Let Λ be a bounded open set and let Λ' be open with $\bar{\Lambda} \subset \Lambda'$. Let $m > j$. Then the map of $H^m(\Lambda')$ into $H^j(\Lambda)$ by restriction is compact.

Proof Pick $\eta \in C_0^\infty(\Lambda')$ with $\eta \equiv 1$ on Λ. Given a sequence $\{f_k\}$ in $H^m(\Lambda')$ with $\|f_k\|_m \leq 1$ let $g_k \equiv \eta f_k$. Then, it is easy to see that $\|g_k\|_m \leq c$ for some fixed c. Moreover, each g_k lies in $H_0^m(\Lambda')$. As a result, we can find a subsequence $g_{k(i)}$ converging in $H_0^j(\Lambda')$. But then $g_{k(i)} \restriction \Lambda \equiv f_{k(i)} \restriction \Lambda$ converges in $H^j(\Lambda)$. ∎

Corollary 1 Let $-\Delta$ denote the Laplacian on $\mathbb{R}^m$ and let u_n be a sequence of functions in $Q(-\Delta)$ satisfying $\|\nabla u_n\| \leq c$, $\|u_n\| \leq c$ for some c. Then, given $R > 0$, u_n has a subsequence converging in the norm $(\int_{|x| \leq R} |v(x)|^2 \, dx)^{1/2}$. Similarly, given $u_n \in D(-\Delta)$ with $\|\nabla u_n\| \leq c$, $\|-\Delta u_n\| \leq c$, then u_n has a subsequence converging in the seminorm $(\int_{|x| \leq R} |\nabla v(x)|^2 \, dx)^{1/2}$.

Proof Choose $\Lambda = \{x \mid |x| \leq R\}$ and $\Lambda' = \mathbb{R}^m$. Since $Q(-\Delta) = H^1(\mathbb{R}^m)$ and $\|u\|_{H^1(\mathbb{R}^m)} \leq \|\nabla u\|_{L^2} + \|u\|_{L^2}$, the first part follows from Theorem XIII.74. The second part follows from the first if we note that $\|\nabla \partial_i u\| \leq \|\Delta u\|$ since we can pass to the Fourier transform and use the fact that $\sum_j (k_j k_i)^2 \leq k^4$. ∎

The above corollary is needed in the study of scattering by inhomogeneous media using the Lax–Phillips method (Section XI.11). For scattering off an obstacle with Dirichlet boundary conditions, one needs instead the following corollary. The proof, which is a little longer, is outlined in Problem 124.

Corollary 2 Let K be a compact subset of $\mathbb{R}^m$ and let $-\Delta_D$ denote the Dirichlet Laplacian on $L^2(\mathbb{R}^m \backslash K)$. Let u_n be a sequence of functions in $Q(-\Delta_D)$ with $(u_n, (-\Delta_D)u_n) \leq c^2$, $\|u_n\| \leq c$ for some c. Then, given $R > 0$, $\{u_n\}$ has a subsequence converging in the norm $(\int_{\{x \mid |x| \leq R\} \backslash K} |v(x)|^2 \, dx)^{1/2}$. Similarly, given $u_n \in D(-\Delta_D)$ with $\|-\Delta_D u_n\| \leq c$ and $(u_n, (-\Delta_D)u_n) \leq c^2$, then, if $m \geq 3$, $\{u_n\}$ has a subsequence converging in the seminorm

$$\left(\int_{\{x \mid |x| \leq R\} \backslash K} |\nabla v(x)|^2 \, dx \right)^{1/2}$$

The case of Neumann boundary conditions is more subtle.

Example 2 Let $\Gamma_1, \ldots, \Gamma_n, \ldots$ be an infinite sequences of disjoint open balls with radii decreasing so fast that $\Lambda = \bigcup \Gamma_i$ is bounded. Let f_i be the function that is that positive multiple of the characteristic function of Γ_i with $\|f_i\| = 1$ in $L^2(\Lambda)$. Then the f_i are an orthonormal set in each $H^m(\Lambda)$ so that $H^m(\Lambda)$ is not compactly embedded in $H^j(\Lambda)$ for any m or j.

While this example is somewhat artificial since Λ is not connected, it is reasonably clear that one should be able to join the Γ's with extremely narrow "corridors" without destroying the noncompactness of the embeddings. In general compactness results for the embedding $H^m(\Lambda) \subset H^j(\Lambda)$ depend on very subtle geometric properties of Λ. We shall settle for stating one of the stronger results.

Definition Let Λ be a bounded open set in $\mathbb{R}^m$ and let $\partial\Lambda \equiv \bar{\Lambda} \backslash \Lambda$ be its topological boundary. Λ is said to have the **segment property** if $\partial\Lambda$ has a finite open covering $\{O_i\}$ and corresponding nonzero vectors $\{y_i\}$ so that for $0 < t < 1$, $x + ty_i$ is in Λ if $x \in \bar{\Lambda} \cap O_i$.

Let us illustrate the definition by some examples in $\mathbb{R}^2$. First, it is clear that if $\partial\Lambda$ is a smooth curve, then Λ has the segment property. Also, if Λ is bounded by finitely many smooth curves that meet at nonzero angles, then Λ will have the segment property. The arcs in Figure XIII.7 can even meet in

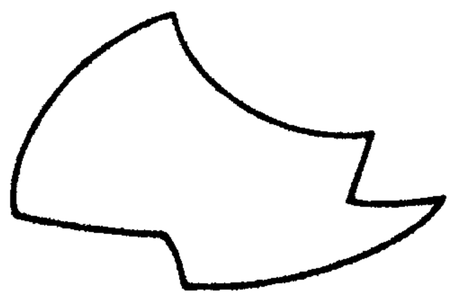


FIGURE XIII.7 A domain with the segment property.

cusps and retain the segment property as long as the cusps are not too wiggly (Figure XIII.8). The canonical example of a nice region without the segment property is a disk with a line segment removed (see Figure XIII.9).

References for the following compact embedding theorem are given in the notes.



(a) A smooth cusp (b) A wiggly cusp

FIGURE XIII.8

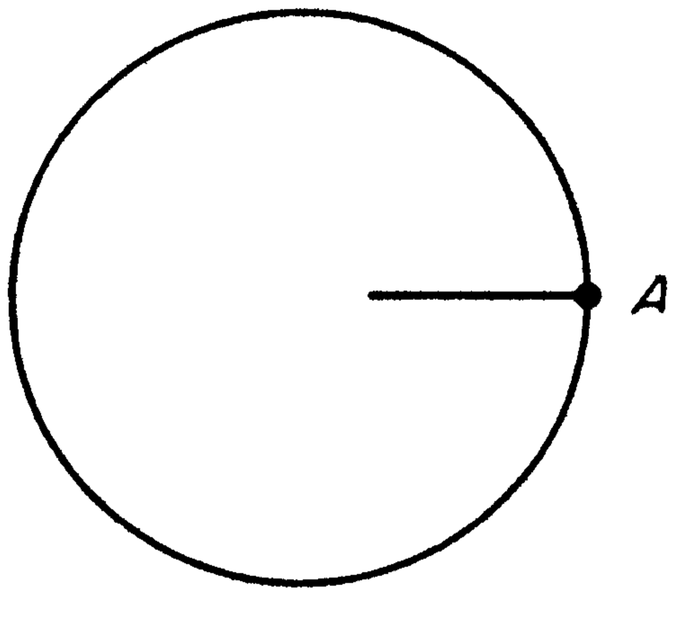


FIGURE XIII.9 The point A destroys the segment property.

Theorem XIII.75 Let Λ be a bounded open set having the segment property. Then $H^m(\Lambda)$ is compactly embedded in $H^j(\Lambda)$ for $m > j$.

By following the proof of the corollary to Theorem XIII.73, we immediately conclude:

Corollary 1 Let Ω be a bounded open region in $\mathbb{R}^m$ obeying the segment property. The Neumann Laplacian $-\Delta_N^\Omega$ has compact resolvent.

Corollary 2 Let K be a compact subset of $\mathbb{R}^m$ and suppose that $\mathbb{R}^m \backslash K$ obeys the segment property in the sense that it holds for $\mathscr{B}_{R_0} \backslash K$ where $\mathscr{B}_{R_0}$ is some open ball containing K. Let $-\Delta_N$ denote the Neumann Laplacian on $L^2(\mathbb{R}^m \backslash K)$ and suppose that $u_n \in Q(-\Delta_N)$ is a sequence of functions so that $\|u_n\| \leq c$ and $(u_n, (-\Delta_N)u_n) \leq c^2$ for some c. Then for each $R > 0$, $\{u_n\}$ has a subsequence that converges in the norm $(\int_{\{x \mid |x| \leq R\} \backslash K} |v(x)|^2 \, dx)^{1/2}$. Similarly, if $u_n \in D(-\Delta_N)$ and $\|-\Delta_N u_n\| \leq c$, $(u_n, (-\Delta_N)u_n) \leq c^2$, then $\{u_n\}$ has a subsequence converging in the seminorm $(\int_{\{x \mid |x| \leq R\} \backslash K} |\nabla v(x)|^2 \, dx)^{1/2}$.

The reader is asked to deduce Corollary 2 from Theorem XIII.75 in Problem 124.

* * *

Another situation where operators with compact resolvent enter naturally is in the study of quantum statistical mechanical systems in boxes. Let Ω be a bounded open subset of $\mathbb{R}^3$. For an N-particle system, let $\Omega_N = \Omega \times \cdots \times \Omega \subset \mathbb{R}^{3N}$ and let $\mathscr{H} = L^2(\Omega_N, d^{3N}x)$. If one wishes to deal with particles obeying Bose–Einstein statistics or Fermi–Dirac statistics, one needs to take the Hilbert space to be $\mathscr{H}_s$, the space of all symmetric functions, or $\mathscr{H}_a$, the space of antisymmetric functions. All the results that we discuss here go through without change. Let H_0 denote the Friedrichs extension of $-\Delta$ on $C_0^\infty(\Omega_N)$. H_0 is the total kinetic energy. Let W be an infinitesimally small form perturbation of $-\Delta$ on $\mathbb{R}^3$, say $W \in R$, the Rollnik class, and let

$$V = \sum_{1 \leq i < j \leq N} W(\mathbf{r}_i - \mathbf{r}_j)$$

as a multiplication operator on $\mathscr{H}$. Then it is not hard to see that V is an infinitesimal form perturbation of H_0 (Problem 122). The first step in studying statistical mechanical systems is:

Theorem XIII.76 The above operator $H = H_0 + V$ has compact resolvent. Moreover, for any $\beta > 0$, $e^{-\beta H}$ is trace class.

Proof Since V is a form bounded perturbation with relative bound zero, it is easy to see that, for any $\varepsilon > 0$, there is a c with

$$(1 - \varepsilon)(H_0 - c) \leq H \leq (1 + \varepsilon)(H_0 + c)$$

so that

$$(1-\varepsilon)[\mu_n(H_0)-c] \leq \mu_n(H) \leq (1+\varepsilon)(\mu_n(H_0)+c) \tag{110}$$

From (110) and Theorem XIII.64, we see that H has compact resolvent if and only if H_0 does. Notice that $e^{-\beta A}$ is trace class if and only if $\sum_{n=1}^{\infty} e^{-\beta\mu_n(A)} < \infty$. Thus, again using (110), $e^{-\beta H}$ is trace class for all positive β if and only if $e^{-\beta H_0}$ is trace class for all positive β. So we have reduced the proof to the case $V = 0$. Make the Ω_N dependence of H_0 explicit by writing $H_0(\Omega_N)$. Since, by definition of the Friedrichs extension, $C_0^\infty(\Omega_N)$ is a form core for $H_0(\Omega_N)$, and since $C_0^\infty(\Omega) \subset C_0^\infty(\Omega')$ if $\Omega \subset \Omega'$, by the min–max principle we see that

$$\mu_n(H_0(\Omega)) \geq \mu_n(H_0(\Omega'))$$

if $\Omega \subset \Omega'$. Any Ω_N can be inbedded in a box $\Omega' \subset \mathbb{R}^{3N}$, so we need just show

$$\sum_n \exp(-\beta\mu_n[H_0(\Omega')]) < \infty \tag{111}$$

If Ω' has sides $\ell_1, \ldots, \ell_{3N}$, its eigenvalues are just

$$E_{m_1,\ldots,m_{3N}} \equiv \sum_{i=1}^{3N} m_i^2(\pi/\ell_i)^2$$

where $m_1, \ldots, m_{3N}$ are arbitrary positive integers. Let $a = \min\{(\pi/\ell_i)^2 \,|\, i = 1, \ldots, 3N\}$. Then $E_{m_1,\ldots,m_{3N}} \geq a\sum_{i=1}^{3N} m_i^2 \geq a\sum_{i=1}^{3N} m_i$ so that

$$\sum_n \exp(-\beta\mu_n[H_0(\Omega')]) \leq \sum_{m_i \geq 1} \exp\left(-\beta a \sum_{i=1}^{3N} m_i\right)$$

$$= \left[\sum_{m=1}^{\infty} \exp(-\beta a m)\right]^{3N} < \infty$$

since the geometric series is convergent. This proves (111) and the theorem. ∎

The above theorem is just the start of the discussion of quantum statistical mechanics. For further discussion, see the reference in the Notes.

What we have discussed thus far in this section relates compactness and discreteness of the entire spectrum. We conclude by giving conditions on a self-adjoint operator guaranteeing that a part of its spectrum is discrete.

Theorem XIII.77 Let A be a self-adjoint operator. Then the part of spectrum of A in (a, b) is purely discrete if and only if $f(A)$ is compact for every continuous function f with $\operatorname{supp} f \subset (a, b)$.

Proof Let supp $f \subset [c, d]$, $a < c \leq d < b$. If A has purely discrete spectrum in (a, b), then there are only finitely many points $\lambda_1, \ldots, \lambda_n \in \sigma(A) \cap [c, d]$ since no point in $[c, d]$ is a limit point of $\sigma(A)$. Moreover, each spectral projection $P(\lambda_i)$ is finite dimensional. Thus

$$f(A) = \sum_{i=1}^{n} f(\lambda_i) P(\lambda_i)$$

is an operator vanishing on the orthogonal complement of a finite-dimensional space and so it is compact.

Conversely, let each $f(A)$ with supp $f \subset (a, b)$ be compact. Let $[c, d] \subset (a, b)$. Let f be a positive continuous function with $0 \leq f \leq 1$, $f(x) = 1$ if $c \leq x \leq d$ and supp $f \subset (a, b)$. Then $P([c, d])$, the spectral projection for $[c, d]$ obeys $P([c, d]) f(A) = P([c, d])$ so it is compact. Therefore, it has finite-dimensional range so that any $\lambda \in [c, d]$ is either in $\rho(A)$ or $\sigma_{\text{disc}}(A)$. ∎

Two important corollaries of Theorem XIII.77 are:

Corollary 1 Let A_n be a sequence of self-adjoint operators with purely discrete spectrum in an interval (a, b). Let A_n converge to A in norm resolvent sense. Then A has purely discrete spectrum in (a, b).

Proof By Theorem VIII.20, if f is continuous with support in (a, b), then $f(A_n) \to f(A)$ in norm. Since a norm limit of compact operators is compact, the theorem follows from Theorem XIII.77. ∎

Corollary 2 Let A_n be a sequence of self-adjoint operators with $\sigma_{\text{ess}}(A_n) = [\Sigma_n, \infty)$. Suppose that $A_n \to A$ in norm resolvent sense. Then Σ_n converges as $n \to \infty$ to some Σ (possibly ∞) and $\sigma_{\text{ess}}(A) = [\Sigma, \infty)$.

Proof By passing to a subsequence, we may suppose that $\Sigma_n \to \Sigma$. By Corollary 1, $\sigma_{\text{ess}}(A) \subset [\Sigma, \infty)$ and by Theorem VIII.23, $(\Sigma, \infty) \subset \sigma_{\text{ess}}(A)$. Thus $\sigma_{\text{ess}}(A) = [\Sigma, \infty)$. In particular, $\inf \sigma_{\text{ess}}(A)$ is the only possible limit point of the original sequence Σ_n so Σ_n converges. ∎

XIII.15 The asymptotic distribution of eigenvalues

We know a great deal more about the forces which produce the vibrations of sound than about those which produce the vibrations of light. To find out the different tunes sent out by a vibrating system is a problem which may or may not be solvable in certain special cases, but it would baffle the most skilful mathematician to solve the inverse problem and to find out the shape of a bell by means of the sounds which it is capable of sending out. And this is the problem which ultimately spectroscopy hopes to solve in the case of light. In the meantime we must welcome with delight even the smallest step in the desired direction.

A. Schuster, 1882

In this section we describe a method for obtaining qualitative information about point spectra. This method has its roots in classical mathematical physics where one wants to know the asymptotic behavior as $\lambda \to \infty$ of the function $N(\lambda) = \dim P_{(-\infty, \lambda)}(A)$ where A is a self-adjoint operator that arises in a boundary value problem. The most famous example of such a result is Weyl's proof that for $-\Delta$ with Dirichlet boundary conditions in a bounded region $\Omega \subset \mathbb{R}^m$, $N(\lambda)$ is asymptotically equal to $C_m \lambda^{m/2}$ times the volume of Ω, where C_m is the m-dependent constant

$$C_m = [m 2^{m-1} \pi^{m/2} \Gamma(\tfrac{1}{2}m)]^{-1}$$

with $\Gamma(\cdot)$ the Euler gamma function; explicitly

$$\Gamma(\tfrac{1}{2}m) = \begin{cases} (k-1)! & (m = 2k) \\ 2^{-2k}(2k)!\,\pi^{1/2}/k! & (m = 2k+1) \end{cases}$$

where k is an integer.

The method we develop will also be used to answer quantum-mechanical questions such as: If $-\Delta + V$ has compact resolvent, how rapidly does $\dim P_{(-\infty, E)}(-\Delta + V)$ grow as $E \to \infty$? If V is a potential going to zero at infinity but so slowly that $\dim P_{(-\infty, 0)}(-\Delta + V) = \infty$, how rapidly does $\dim P_{(-\infty, E)}(-\Delta + V)$ grow as $E \uparrow 0$? If W is a short-range potential, what is the rate of growth of $\dim P_{(-\infty, 0)}(-\Delta + \lambda W)$ as $\lambda \to \infty$? Elements of this technique have also proven useful in studying the pressure in quantum statistical mechanics, the Fock space energy per unit volume in constructive field theory, and the validity of the Thomas–Fermi model in atomic physics.

There is associated with these problems an intuition that is critical for understanding the structure of the machinery we shall develop. Consider first Weyl's result. The constant C_m is not really as unpleasant or unnatural as it looks. If τ_m is the volume of the unit ball in $\mathbb{R}^m$, then $C_m = \tau_m/(2\pi)^m$. Thus the asymptotic value of $N(\lambda)$ is

$$N(\lambda) \sim (\tau_m \lambda^{m/2})(\text{vol } \Omega)/(2\pi)^m$$

so in some sense $N(\lambda)$ appears to be associated with a volume in $\mathbb{R}^{2m}$ (instead of $\mathbb{R}^m$ as one might guess directly from the formula $C_m(\text{vol } \Omega)$). In fact, since $\tau_m \lambda^{m/2} = \text{vol}\{p \in \mathbb{R}^m \mid p^2 < \lambda\}$, we see that

$$N(\lambda) \sim \text{vol}\{\langle x, p\rangle \mid x \in \Omega,\ p^2 < \lambda\}/(2\pi)^m$$

Thus $(2\pi)^m N(\lambda)$ is asymptotic to the volume of the region of phase space where a classical particle of mass $m = \frac{1}{2}$, moving freely within Ω (with, for example, elastic collisions with the wall), has energy $E_{\text{class}} \leq \lambda$. In units with $\hbar = 1$, $-\Delta_D$, the Laplacian with Dirichlet boundary conditions in Ω, is just

the quantum energy corresponding to the classical free particle in Ω. Thus, we see that as $\lambda \to \infty$, the number of quantum states is given by a classical phase space volume divided by $(2\pi)^m$. This is in agreement with the "old quantum theory" Bohr–Sommerfeld quantization condition that each quantum state is associated with a volume of h^m in phase space since $h \equiv 2\pi\hbar = 2\pi$ in our units. It is an interesting historical accident that Weyl's result was approximately contemporary to the work of Bohr and Sommerfeld although the connection was not completely realized until some years afterward. The results we shall prove for the quantum questions mentioned above will all have the interpretation of a phase space volume divided by $(2\pi)^n$. Thus, for example, for W short range,

$$(2\pi)^{-m} \operatorname{vol}\{\langle p, x\rangle \mid p^2 + \lambda W(x) < 0\} = \frac{\tau_m}{(2\pi)^m} \int_{\{x \mid W(x) < 0\}} \lambda^{m/2} \mid W(x) \mid^{m/2} d^m x$$

which is asymptotically the expression which we shall obtain for $\dim P_{(-\infty, 0)}(-\Delta + \lambda W)$.

The idea of the method that we shall use to study the above problems is quite simple and is connected to the phase space intuition just described. For cubes, the eigenvalues of the Laplacian with Dirichlet boundary conditions $(-\Delta_D)$ or Neumann boundary conditions $(-\Delta_N)$ can be computed explicitly and the asymptotic formula of Weyl can be directly verified (Proposition 2); the content of the formula in this case is essentially the statement that the volume of a large ball in $\mathbb{R}^m$ is approximately the number of points in it whose coordinates are integral. When Ω is a union of cubes (together with any common boundaries) the formula of Weyl is much subtler but the fact that phase space volumes "are local in x space," i.e., that according to Weyl, $N(\lambda; \Omega_1 \cup \Omega_2)$ is asymptotically equal to $N(\lambda; \Omega_1) + N(\lambda; \Omega_2)$ suggests that we try to decouple the cubes in Ω along their common boundary and use the fact that we know how to control individual cubes. Here a rather remarkable fact about boundary conditions helps us. There are two operators that we can compare with $-\Delta_D^\Omega$. One operator has added Dirichlet boundary conditions on the common boundaries, call it $-\tilde{\Delta}_D$, and the other has added Neumann boundary conditions, $-\tilde{\Delta}_N$. There is decoupling in $-\tilde{\Delta}_D$ in the sense that $-\tilde{\Delta}_D = \bigoplus_\alpha (-\Delta_D^{\Omega_\alpha})$ (and similarly for N) where Ω is the union of cubes Ω_α together with common boundary (Theorem XIII.79). Moreover one can sandwich $N(\lambda; -\Delta_D^\Omega)$ between $N(\lambda; -\tilde{\Delta}_D)$ and $N(\lambda; -\tilde{\Delta}_N)$, i.e., $N(\lambda; -\tilde{\Delta}_D) \leq N(\lambda; -\Delta_D^\Omega) \leq N(\lambda; N\tilde{\Delta}_N)$. We shall refer to this combined method of decoupling and monotonicity as **Dirichlet–Neumann bracketing**.

We begin our formal discussion with a study of Dirichlet and Neumann boundary conditions.

Definition Let Ω be an open region of $\mathbb{R}^m$ with connected components $\Omega_1, \ldots$ (finite or infinite). The **Dirichlet Laplacian for Ω**, $-\Delta_D^\Omega$, is the unique self-adjoint operator on $L^2(\Omega, d^m x)$ whose quadratic form is the closure of the form $q(f, g) = \int \overline{\nabla f} \cdot \nabla g \, d^m x$ with domain $C_0^\infty(\Omega)$. The **Neumann Laplacian for Ω**, $-\Delta_N^\Omega$, is the unique self-adjoint operator on $L^2(\Omega, d^m x)$ whose quadratic form is $q(f, g) = \int \overline{\nabla f} \cdot \nabla g \, d^m x$ on the domain

$$H^1(\Omega) = \{f \in L^2(\Omega) \,|\, \nabla f \in L^2(\mathbb{R}^m)\}$$

where by ∇f we mean the distributional gradient, i.e.,

$$\int (\nabla f)\varphi \, dx = -\int f(\nabla \varphi) \, dx$$

for all $\varphi \in C_0^\infty(\mathbb{R}^m)$. When a fixed Ω is intended, we shall drop the superscript Ω.

There are various alternative descriptions of $-\Delta_D^\Omega$ and $-\Delta_N^\Omega$. Clearly, $-\Delta_D^\Omega$ is the Friedrichs extension by definition, and therefore $Q(-\Delta_D^\Omega)$ is the space $H_0^1(\Omega)$ defined in the preceding section. It follows from our discussion there that

$$\{f \in H^1(\Omega) \,|\, \text{supp } f \text{ is compact in } \Omega\}$$

is contained in $Q(-\Delta_D^\Omega)$. For any Ω, one also has the following description: Let D denote the *operator* closure of the gradient on $C_0^\infty(\Omega)$. Then $-\Delta_D^\Omega = D^*D$ while $-\Delta_N^\Omega = DD^*$. For nice regions, in particular for those obeying the segment condition,

$$\{f \in H^1(\Omega) \,|\, f \text{ is } C^\infty \text{ up to } \partial\Omega\}$$

is a form core for $-\Delta_N^\Omega$. If Ω has a nice boundary, $-\Delta_D$ has an *operator* core functions that are C^∞ up to $\partial\Omega$ and that vanish on $\partial\Omega$, and $-\Delta_N$ has an *operator* core functions that are C^∞ up to $\partial\Omega$ and whose normal derivatives vanish on $\partial\Omega$. It is this last description that is responsible for the names "Dirichlet" and "Neumann" after the classical boundary value problems of potential theory. For the case of cubes, we shall need this last description.

Proposition 1 Let Ω be a cube in $\mathbb{R}^m$. Then:

(a) $D_D \equiv \{f \mid f \text{ is } C^\infty \text{ up to } \partial\Omega \text{ with } f \restriction \partial\Omega = 0\}$ is an operator core for $-\Delta_D$ and for $f \in D_D$,

$$-\Delta_D f = -\sum_{i=1}^{m} \frac{\partial^2 f}{\partial x_i^2}$$

(b) $D_N \equiv \{f \mid f \text{ is } C^\infty \text{ up to } \partial\Omega \text{ with } \partial f/\partial n \restriction \partial\Omega = 0\}$ is an operator core for $-\Delta_N$ and for such f,

$$-\Delta_N f = -\sum_{i=1}^{m} \frac{\partial^2 f}{\partial x_i^2}$$

Here $\partial/\partial n$ denotes the normal derivative at the boundary.

Proof (a) Without loss of generality, let $\Omega = (-1, 1)^m$. Let A denote the operator $-\Delta$ with domain D_D. We wish to show that $-\Delta_D = \bar{A}$. A is clearly symmetric, and by separation of variables (multiple Fourier series) we can find a complete orthonormal basis of eigenfunctions $\{\varphi_n\}$ for A. If $A\varphi_n = \lambda_n \varphi_n$, it is easy to see that $\varphi \in D(\bar{A})$ if and only if $\sum \lambda_n^2 |(\varphi_n, \varphi)|^2 < \infty$; and from this we conclude that $\bar{A}$ is self-adjoint.

Clearly, $C_0^\infty(\Omega) \subset D(\bar{A}) \subset Q(\bar{A})$ and as quadratic forms $A \restriction C_0^\infty(\Omega) \times C_0^\infty(\Omega) = -\Delta_D \restriction C_0^\infty(\Omega) \times C_0^\infty(\Omega)$, so it is sufficient to prove that $Q(\bar{A}) \subset Q(-\Delta_D)$. Since $D_D = D(A)$ is a form core for $\bar{A}$ as a quadratic form, we need only prove that $D_D \subset Q(-\Delta_D)$. Thus it suffices to find for each $f \in D_D$ a sequence $f_n \in C_0^\infty(\Omega)$ with $\|f_n - f\| + \|\nabla f_n - \nabla f\| \to 0$. Given $f \in D_D$, let $g_n(x) = f((1 + n^{-1})x)$ if $|x_i| \leq (1 + n^{-1})^{-1}$ and zero otherwise. Then $g_n(x)$ is continuous and piecewise C^1 with bounded gradient. Moreover, $g_n \to f$ and $\nabla g_n \to \nabla f$ in L^2. Let $j_\delta(x)$ be an approximate identity. Then $g_n * j_\delta \to g_n$ and $\nabla(g_n * j_\delta) \to \nabla g_n$ as $\delta \to 0$. Since $g_n * j_\delta \in C_0^\infty(\Omega)$ for δ small, we can find a suitable sequence $\{f_n\}$.

(b) Assume that $\Omega = (-1, 1)^m$. Let B denote the operator $-\Delta$ with domain D_N. As in part (a), B is easily seen to be essentially self-adjoint by looking at its eigenfunctions. Moreover, since $D(B) \subset H^1(\Omega)$ and $(f, Bf) = \int |\nabla f|^2 \, d^2x$ for $f \in D(B)$ (by the boundary condition), we have $Q(\bar{B}) \subset Q(-\Delta_N)$, so that it is sufficient to prove that $Q(-\Delta_N) \subset Q(\bar{B})$. To show this, it is enough to prove that $H^1(\Omega) \subset Q(\bar{B})$.

Let f be in $H^1(\Omega)$. We first claim that if g and ∇g are continuous up to the boundary and $g(\pm 1, x_2, \ldots, x_m) = 0$, then

$$(\partial_1 f, g) = -(f, \partial_1 g) \tag{112}$$

Suppose first that g vanishes on all of $\partial\Omega$. Then, as in the proof of (a) we can find $g_n \in C_0^\infty(\Omega)$ so that $g_n \to g$, $\nabla g_n \to g$ so that (112) follows since it holds for $g = g_n$. Now, let η_n be a sequence of C^∞ functions on Ω depending only on $x_2, \ldots, x_m$ with compact support in

$$\{x \,|\, |x_2| \leq 1 - n^{-1}, \ldots, |x_m| \leq 1 - n^{-1}\}$$

such that $\eta_n(x) \uparrow 1$ as $n \to \infty$. Then (112) holds for $g\eta_n$ and thus for g also since $\partial_1(g\eta_n) = \eta_n\, \partial_1 g$.

Let $\{\psi_n\}$ be the eigenfunctions for B given by (115) below. By replacing $\sin(n_1 \pi x/2)$ by $\cos(n_1 \pi x/2)$ when n_1 is odd and $\cos(n_1 \pi x/2)$ by $\sin(n_1 \pi x/2)$ when n_1 is even, we can find an orthonormal family $\{\varphi_n\}_{n_1 \geq 1}$ so that $\partial_1 \varphi_n = \pm(\pi/2) n_1 \psi_n$. The functions φ_n and $\nabla\varphi_n$ are continuous up to the boundary and $\varphi_n(\pm 1, x_2, \ldots, x_m) = 0$. Using (112), we find

$$\sum_n |(f, \psi_n)|^2 n_1^2 = \left(\frac{2}{\pi}\right)^2 \sum_n |(\partial_1 f, \varphi_n)|^2$$

$$\leq \left(\frac{2}{\pi}\right)^2 \|\partial_1 f\|_2^2$$

since the φ_n are orthonormal. Doing a similar procedure in each variable, we conclude that

$$\sum_n (1 + n^2) |(f, \psi_n)|^2 \leq \|f\|_2^2 + \left(\frac{2}{\pi}\right)^2 \|\nabla f\|_2^2$$

so $f \in Q(\bar{B})$. ∎

At first sight it seems surprising that the operator $-\Delta_N^\Omega$ which we have defined in a way that makes no mention of $\partial\Omega$ or normal derivatives should obey Neumann boundary conditions. On an intuitive level, one can understand this in several ways. Since $-\Delta_N^\Omega = DD^*$, for f to be in the domain of $-\Delta_N^\Omega$, we need D^*f to be in the domain of D. And, intuitively, the domain of D consists of functions that vanish on $\partial\Omega$.

The second intuition is clearest in one dimension so let $\Omega = (a, b)$. The operator C defined by the Neumann quadratic form should be a self-adjoint extension of $-d^2/dx^2$ on $C_0^\infty(a, b)$ satisfying two properties:

(i) For any function f that is C^∞ on $[a, b]$, there should be a sequence $f_n \in D(C)$ so that $f_n \to f$ in H^1.
(ii) For any $f \in D(C)$, $(f, Cf) = \|df/dx\|^2$.

We could not impose Dirichlet conditions on C because that would require us to make the f_n vanish at a and b, which would require that $d(f_n - f)/dx$ be large near the end points. This would also rule out periodic boundary conditions that link the two end points. However, condition (i) does not rule out boundary conditions of the form $df/dx + \alpha f = 0$. Condition (ii) forces α to be zero (Problem 127).

The main advantage of the above characterization is that it provides explicit eigenvalues and eigenvectors of $-\Delta_D$ and $-\Delta_N$. To label them we denote the nonnegative integers by $\mathbb{Z}_+$ and the strictly positive integers as $\mathbb{Z}_{++}$, so $\mathbb{Z}_+ = \mathbb{Z}_{++} \cup \{0\}$. Then the eigenvectors and eigenvalues of $-\Delta_D$ in $(-a, a)^m$ are labeled by $\mathbb{Z}_{++}^m$ with eigenvectors

$$\Phi_{n;a}(x) = a^{-m/2} \prod_{i=1}^{m} \varphi_{n_i}(x_i/a) \tag{113}$$

where

$$\varphi_k(x) = \cos(k\pi x/2); \qquad k = 1, 3, 5, \ldots$$

$$\varphi_k(x) = \sin(k\pi x/2); \qquad k = 2, 4, 6, \ldots$$

and eigenvalues

$$E_n(a) = \left(\frac{\pi}{2a}\right)^2 \sum_{i=1}^{m} n_i^2 \tag{114}$$

For $-\Delta_N$ in $(-a, a)^m$, the eigenvectors are labeled by $\mathbb{Z}_+^m$ with eigenvectors

$$\Psi_{n;a}(x) = a^{-m/2} \prod_{i=1}^{m} \psi_{n_i}(x_i/a) \tag{115}$$

where

$$\psi_k(x) = \sin(k\pi x/2); \qquad k = 1, 3, 5, \ldots$$

$$\psi_k(x) = \cos(k\pi x/2); \qquad k = 2, 4, 6, \ldots$$

$$\psi_k(x) = \tfrac{1}{2}\sqrt{2}; \qquad k = 0$$

and with eigenvalues still given by (114). Because of this explicit listing, one can prove Weyl's theorem directly for cubes.

Proposition 2 Let $N_D(a, \lambda)$ (respectively, $N_N(a, \lambda)$) denote the dimension of the spectral projection $P_{[0,\lambda)}$ for $-\Delta_D$ (respectively, $-\Delta_N$) on $(-a, a)^m$.

Then for all a, λ, we have

$$|N_D(a, \lambda) - \tau_m(2a/2\pi)^m\lambda^{m/2}| \leq C(1 + (a^2\lambda)^{(m-1)/2}) \tag{116}$$

and

$$|N_N(a, \lambda) - \tau_m(2a/2\pi)^m\lambda^{m/2}| \leq C(1 + (a^2\lambda)^{(m-1)/2}) \tag{117}$$

where τ_m is the volume of the unit ball in $\mathbb{R}^m$ and C is a suitable constant.

Proof We begin with two remarks. The first explains why the result is true. On account of (114) N_D (respectively, N_N) is the number of points of $\mathbb{Z}^m_{+\,+}$ (respectively, $\mathbb{Z}^m_+$) within a ball of radius $(2a/\pi)\lambda^{1/2}$. For large λ, this should be approximately the volume of an "octant" of this sphere, i.e., $2^{-m}\tau_m((2a/\pi)\lambda^{1/2})^m$. The error should be a "surface term," i.e., of order $(a^2\lambda)^{(m-1)/2}$. The second remark is to note that $-\Delta_D$ in $(-1, 1)^m$ is unitarily equivalent under scaling to $a^2(-\Delta_D)$ in $(-a, a)^m$, so $N_D(a, \lambda) = N_D(1, a^2\lambda)$. As a result, we need only prove the estimates when $a = 1$.

Let S_λ denote the ball of radius $(2/\pi)\lambda^{1/2}$. For each $n \in \mathbb{Z}^m_{+\,+} \cap S_\lambda$, the unit cube $\{x \,|\, n_i - 1 \leq x_i \leq n_i\}$ is contained in the upper octant of S_λ, so

$$N_D(\lambda) \leq \tau_m(2a/2\pi)^m\lambda^{m/2} \tag{118}$$

Since the upper octant of S_λ is covered by the unit cubes $\{x \,|\, n_i \leq x_i < n_i + 1\}$ as n runs through $\mathbb{Z}^m_+ \cap S_\lambda$, we have

$$\tau_m(2a/2\pi)^m\lambda^{m/2} \leq N_N(\lambda) \tag{119}$$

Finally, it is clear that

$$N_N(\lambda) - N_D(\lambda) = \#\{S_\lambda \cap (\mathbb{Z}^m_+ \setminus \mathbb{Z}^m_{+\,+})\} = \bigcup_{k=0}^{m-1} M_k(\lambda)$$

where

$$M_k(\lambda) = \{n \in \mathbb{Z}^m_+ \cap S_\lambda \,|\, \text{exactly } k \text{ of the } n_i \text{ are nonzero}\}$$

(see Figure XIII.10 in case $m = 3$). As in our bound on N_D, $\#(M_k(\lambda))$ is dominated by the k-dimensional volume of $\binom{m}{k}$ octants of $(2/\pi)\lambda^{1/2}$-balls in k space. Therefore,

$$\sum_{k=1}^{m-1} M_k(\lambda) \leq \text{const}\left(\sum_{k=0}^{m-1} \lambda^{k/2}\right) \leq C(1 + \lambda^{(m-1)/2})$$

Thus

$$N_N(\lambda) - N_D(\lambda) \leq C(1 + \lambda^{(m-1)/2}) \tag{120}$$

(118)–(120) clearly imply (116) and (117). ∎

Dirichlet and Neumann Laplacians are useful for analyzing general eigenvalue problems because of two critical properties that occur when a Dirichlet or Neumann surface is added. Consider disjoint Ω_1 and Ω_2 and $\Omega = (\overline{\Omega_1 \cup \Omega_2})^{\text{int}}$ as shown in Figure XIII.11. We shall show below that: (1) Dirichlet and Neumann surfaces decouple (Proposition 3); (2) Dirichlet surfaces raise energies, and Neumann surfaces lower energies (Proposition 4). To be precise about the decoupling we make some preliminary remarks

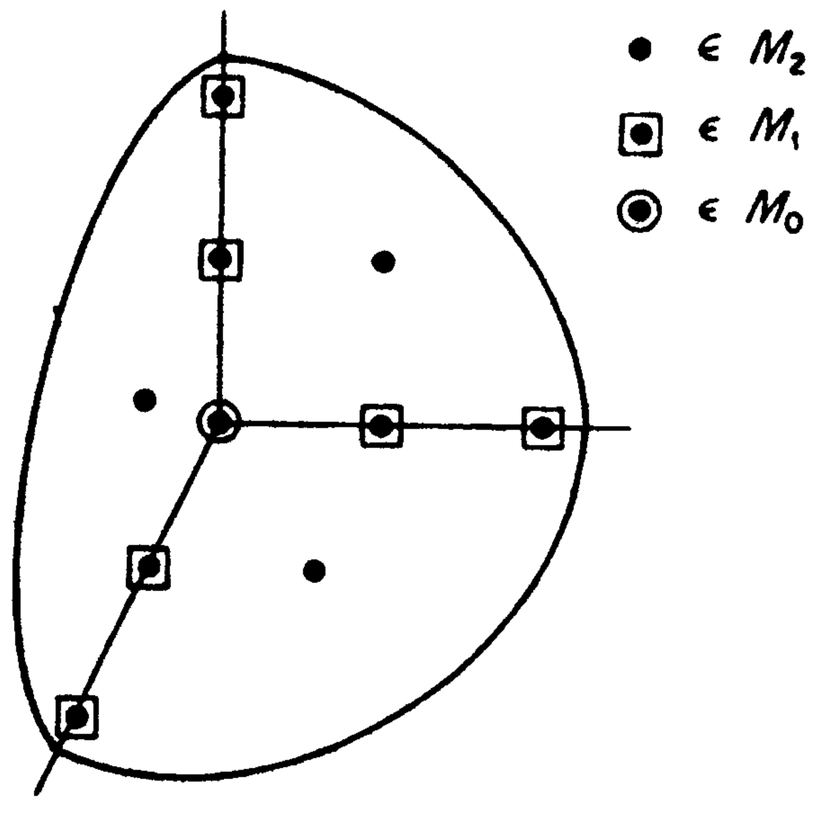


FIGURE XIII.10 The sets M_k.

about direct sums of self-adjoint operators. Let $\mathscr{H} = \mathscr{H}_1 \oplus \mathscr{H}_2$. Let A_1 be a self-adjoint operator on $\mathscr{H}_1$, and A_2 a self-adjoint operator on $\mathscr{H}_2$. Let A be the operator with domain $D(A) = \{\langle \varphi, \psi \rangle \,|\, \varphi \in D(A_1), \psi \in D(A_2)\}$ with $A\langle \varphi, \psi \rangle = \langle A_1 \varphi, A_2 \psi \rangle$. We shall write $A = A_1 \oplus A_2$. There are several properties of $A_1 \oplus A_2$ whose proofs (which use the spectral theorem and/or the fundamental criterion) we leave to the reader (Problem 133):

(1) $A_1 \oplus A_2$ is self-adjoint.

(2) If D_1 is a core for A_1 and D_2 is a core for A_2, then

$$D_1 \oplus D_2 \equiv \{\langle \varphi, \psi \rangle \,|\, \varphi \in D_1, \psi \in D_2\}$$

is a core for $A_1 \oplus A_2$.

(3) $Q(A_1 \oplus A_2) = Q(A_1) \oplus Q(A_2)$; and if $\langle \varphi, \psi \rangle \in Q(A_1) \oplus Q(A_2)$, then

$$(\langle \varphi, \psi \rangle, (A_1 \oplus A_2)\langle \varphi, \psi \rangle) = (\varphi, A_1 \varphi) + (\psi, A_2 \psi)$$

(4) For any Borel subset $\Omega \subset \mathbb{R}$,

$$P_\Omega(A_1 \oplus A_2) = P_\Omega(A_1) \oplus P_\Omega(A_2)$$

(5) If $N(\lambda, A) = \dim P_{(-\infty, \lambda)}(A)$, then

$$N(\lambda, A_1 \oplus A_2) = N(\lambda, A_1) + N(\lambda, A_2)$$

Proposition 3 Let Ω_1 and Ω_2 be disjoint open sets so that $L^2(\Omega_1 \cup \Omega_2) = L^2(\Omega_1) \oplus L^2(\Omega_2)$. Under this decomposition

$$-\Delta_D^{\Omega_1 \cup \Omega_2} = -\Delta_D^{\Omega_1} \oplus -\Delta_D^{\Omega_2}$$

$$-\Delta_N^{\Omega_1 \cup \Omega_2} = -\Delta_N^{\Omega_1} \oplus -\Delta_N^{\Omega_2}$$

Proof We consider the Dirichlet case; the Neumann case is similar. Given $f \in C_0^\infty(\Omega_1 \cup \Omega_2)$, we let $f_i = f \restriction \Omega_i$. Then $f_i \in C_0^\infty(\Omega_i)$ and clearly

$$\int_{\Omega_1 \cup \Omega_2} \overline{\nabla f} \cdot \nabla g \, d^m x = \int_{\Omega_1} \overline{\nabla f_1} \cdot \nabla g_1 \, d^m x + \int_{\Omega_2} \overline{\nabla f_2} \cdot \nabla g_2 \, d^m x$$

Since this relation clearly extends to the closures of the quadratic forms, the quadratic forms are equal so the result follows. ∎

As an example of the use of this proposition we have:

Corollary Let $N_D(\Omega, \lambda)$ (respectively, $N_N(\Omega, \lambda)$) be the dimension of the spectral projection $P_{[0, \lambda)}$ for $-\Delta_D^\Omega$ (respectively, $-\Delta_N^\Omega$). Then if $\Omega_1, \ldots, \Omega_k$ are disjoint,

$$N_D\left(\bigcup_{i=1}^k \Omega_i, \lambda\right) = \sum_{i=1}^k N_D(\Omega_i, \lambda)$$

$$N_N\left(\bigcup_{i=1}^k \Omega_i, \lambda\right) = \sum_{i=1}^k N_N(\Omega_i, \lambda)$$

To state the monotonicity properties, we extend slightly the definition of $A \leq B$ given in Section 2.

Definition Let A and B be self-adjoint operators that are nonnegative where A is defined on a dense subset of a Hilbert space $\mathscr{H}$ and B is defined on a dense subset of a Hilbert subspace $\mathscr{H}_1 \subseteq \mathscr{H}$. We write $0 \leq A \leq B$ if and only if

(i) $Q(A) \supset Q(B)$.
(ii) For any $\psi \in Q(B)$,

$$0 \leq (\psi, A\psi) \leq (\psi, B\psi)$$

The point of this definition is that on account of the min–max principle (in the form of Theorem XIII.2), we immediately have

Lemma If $0 \leq A \leq B$, then:

(a) $\dim P_{[0,\,\lambda]}(A) \geq \dim P_{[0,\,\lambda]}(B)$, all $\lambda > 0$.
(b) $\mu_n(A) \leq \mu_n(B)$ for all n where μ_n is given by the min–max principle.

Proof Since $Q(A)$ contains more trial functions,

$$\min_{\substack{\varphi \in Q(A) \\ \varphi \perp \psi_1, \ldots, \psi_n}} (\varphi, A\varphi) \leq \min_{\substack{\varphi \in Q(B) \\ \varphi \perp \psi_1, \ldots, \psi_n}} (\varphi, A\varphi)$$

$$\leq \min_{\substack{\varphi \in Q(B) \\ \varphi \perp \psi_1, \ldots, \psi_n}} (\varphi, B\varphi)$$

so that (b) holds. (a) follows from (b) and the min–max principle. ∎

Proposition 4

(a) If $\Omega \subset \Omega'$, then $0 \leq -\Delta_D^{\Omega'} \leq -\Delta_D^{\Omega}$.
(b) For any Ω, $0 \leq -\Delta_N^{\Omega} \leq -\Delta_D^{\Omega}$.
(c) Let Ω_1, Ω_2 be disjoint open subsets of an open set Ω so that $\overline{(\Omega_1 \cup \Omega_2)}^{\text{int}} = \Omega$, and $\Omega \backslash \Omega_1 \cup \Omega_2$ has measure 0 (see Figure XIII.11).

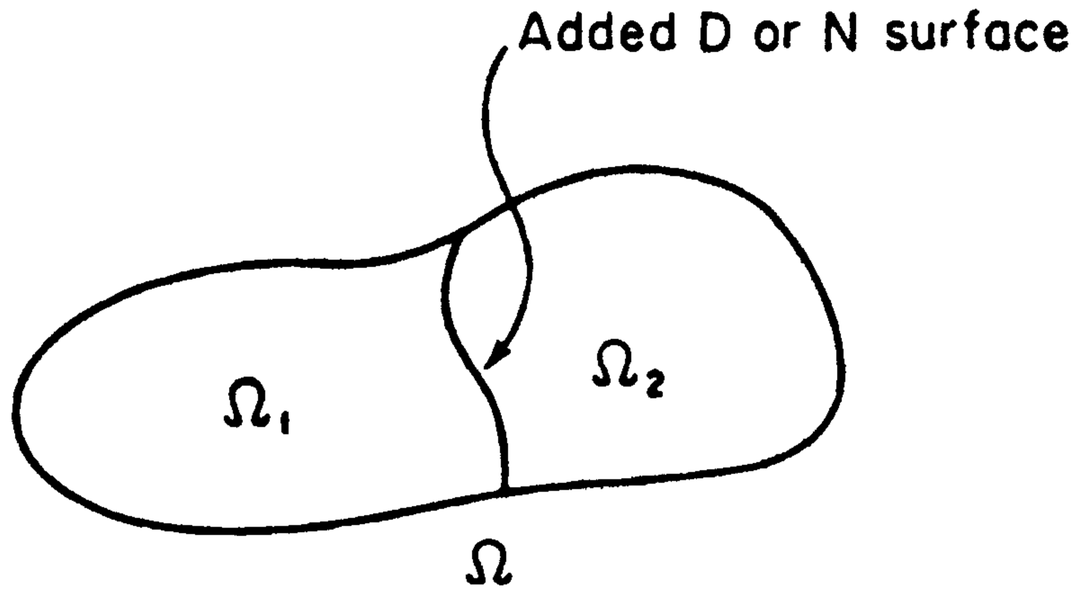


FIGURE XIII.11 Adding a surface.

Then

$$0 \leq -\Delta_D^{\Omega} \leq -\Delta_D^{\Omega_1 \cup \Omega_2}$$

$$0 \leq -\Delta_N^{\Omega_1 \cup \Omega_2} \leq -\Delta_N^{\Omega}$$

Proof (a) This statement is to be interpreted in the sense that any $f \in L^2(\Omega)$ is viewed as an element of $L^2(\Omega')$ by setting it equal to zero in $\Omega' \backslash \Omega$. With this definition, $C_0^\infty(\Omega) \subset C_0^\infty(\Omega')$ and $-\Delta_D^{\Omega'} \restriction C_0^\infty(\Omega) \times C_0^\infty(\Omega) = -\Delta_D^{\Omega}$, as quadratic forms, so (a) follows.

(b) Since $C_0^\infty(\Omega) \subset H^1(\Omega)$, this is immediate.

(c) Clearly $C_0^\infty(\Omega_1 \cup \Omega_2) \subset C_0^\infty(\Omega)$ since $\Omega \supset \Omega_1 \cup \Omega_2$; (indeed, the first part of (c) is a special case of (a)). On the other hand, if $f \in H^1(\Omega)$, its

restriction to $\Omega_1 \cup \Omega_2$ is clearly in $H^1(\Omega_1) \oplus H^1(\Omega_2)$. Moreover, since $\Omega \backslash \Omega_1 \cup \Omega_2$ has measure zero

$$\int_\Omega |\nabla f|^2 \, dx = \int_{\Omega_1 \cup \Omega_2} |\nabla f|^2 \, d^3x \quad \blacksquare$$

The main point about the inequalities in (c) is that by adding an extra Dirichlet "surface" $\Omega \backslash \Omega_1 \cup \Omega_2$, we add an extra requirement on the wave functions (they must vanish on the surface) and so the eigenvalues go up. But it is by *removing* a Neumann "surface" that we add an extra requirement because the functions must be "smooth" across the surface after we remove the boundary condition.

As a first application, we prove the result of Weyl relating the asymptotic density of eigenvalues of $-\Delta_D^\Omega$ and the volume of Ω when Ω is sufficiently nice.

Definition A **standard 2^{-n} cube** in $\mathbb{R}^m$ is a cube of the form

$$\left[\frac{a_1}{2^n}, \frac{a_1 + 1}{2^n}\right) \times \cdots \times \left[\frac{a_m}{2^n}, \frac{a_m + 1}{2^n}\right)$$

in $\mathbb{R}^m$ with $a_1, \ldots, a_m$ integers. Given a set $\Omega \subset \mathbb{R}^m$, we let $W_n^-(\Omega)$ be the volume of those standard 2^{-n} cubes contained in Ω and $W_n^+(\Omega)$ be the volume of standard 2^{-n} cubes that intersect Ω. Thus if Ω is Lebesgue measurable,

$$W_n^-(\Omega) \leq W_{n+1}^-(\Omega) \leq \mu(\Omega) \leq W_{n+1}^+(\Omega) \leq W_n^+(\Omega) \tag{121}$$

The limit $\lim W_n^-(\Omega) = W_\infty^-(\Omega)$ (respectively, $\lim W_n^+(\Omega) = W_\infty^+(\Omega)$) is called the **inner** (respectively, **outer**) **Jordan content** of Ω. If $W_\infty^+(\Omega) = W_\infty^-(\Omega)$, then we say that Ω is a **contented set** and $W(\Omega) = W_\infty^\pm(\Omega)$ is called its **content**.

Notice that by (121) if Ω is both contented and Lebesgue measurable, then $W(\Omega) = \mu(\Omega)$. One can also prove that any contented set is Lebesgue measurable (Problem 128).

Theorem XIII.78 Let Ω be a bounded open set in $\mathbb{R}^m$. Let $N_D(\Omega, \lambda)$ be the dimension of the range of the spectral projection $P_{[0, \lambda)}$ for $-\Delta_D^\Omega$. Then, if Ω is contented,

$$\lim_{\lambda \to \infty} N_D(\Omega, \lambda)/\lambda^{m/2} = \frac{\tau_m}{(2\pi)^m} W(\Omega)$$

Proof We shall show that for any n,

$$\overline{\lim_{\lambda\to\infty}}\, N_D(\Omega, \lambda)/\lambda^{m/2} \leq (2\pi)^{-m}\tau_m W_n^+(\Omega) \tag{122a}$$

$$\underline{\lim_{\lambda\to\infty}}\, N_D(\Omega, \lambda)/\lambda^{m/2} \geq (2\pi)^{-m}\tau_m W_n^-(\Omega) \tag{122b}$$

which implies the result.

Let $\Omega_n^\pm$ denote the union of cubes whose volume enters in the definition of $W_n^\pm(\Omega)$, and let $\{C_{n,\alpha}^\pm\}$ be the interiors of the actual cubes themselves, so that $\bar{\Omega}_n^\pm = \bigcup_\alpha \bar{C}_{n,\alpha}^\pm$. Now, by (a) and (c) of Proposition 4,

$$-\Delta_D^\Omega \leq -\Delta_D^{\Omega n} \leq -\Delta_D^{\bigcup C_{n,\alpha}^-} = \bigoplus_\alpha -\Delta_D^{C_{n,\alpha}^-}$$

where we have used Proposition 3 in the last step. Thus, by Proposition 4,

$$\begin{aligned} N_D(\Omega, \lambda) &\geq \sum_\alpha N_D(C_{n,\alpha}^-, \lambda) \\ &= (\#\alpha) N_D(2^{-n-1}, \lambda) \\ &= W_n^-(\Omega) 2^{nm} N_D(2^{-n-1}, \lambda) \end{aligned}$$

By Proposition 2,

$$\lim_{\lambda\to\infty} N_D(2^{-n-1}, \lambda)\lambda^{-m/2} = \tau_m(2\pi)^{-m}2^{-nm}$$

so (122b) holds. Similarly, by (a)–(c) of Proposition 4,

$$-\Delta_D^\Omega \geq -\Delta_D^{\Omega n^+} \geq -\Delta_N^{\Omega n^+} \geq -\Delta_N^{\bigcup C_{n,\alpha}^+} = \oplus -\Delta_N^{C_{n,\alpha}^+}$$

and (122a) follows by mimicking the steps above. ∎

The structure of the Dirichlet–Neumann bracketing technique is now clear. One uses the monotonicity under addition of Dirichlet or Neumann boundaries and their decoupling properties to reduce a problem to one about cubes which is then solved by Proposition 2. That phase volumes enter is a result of the fact that they enter in (116) and (117). Thus, for example, we have:

Theorem XIII.79 Let V be a continuous function on $\mathbb{R}^m$ that has compact support. Let $N(\lambda)$ be the dimension of the spectral projection $P_{(-\infty, 0)}$ for $-\Delta + \lambda V$. Then

$$\lim_{\lambda\to\infty} N(\lambda)/\lambda^{m/2} = \tau_m(2\pi)^{-m}\int_{\{x|V(x)\leq 0\}} (-V(x))^{m/2}\, d^m x$$

Proof For each n, let $\{C_{n,\alpha}\}_\alpha$ be a listing of all the standard 2^{-n}-cubes. Define V_n^+ (respectively, V_n^-) to be that function piecewise constant over each $C_{n,\alpha}$ with value $\max\{V(x) \mid x \in C_{n,\alpha}\}$ (respectively, $\min\{V(x) \mid x \in C_{n,\alpha}\}$). We shall prove that for each n,

$$\overline{\lim_{\lambda\to\infty}}\, N(\lambda)/\lambda^{m/2} \leq \tau_m(2\pi)^{-m} \int_{\{x \mid V_n^-(x)\leq 0\}} (-V_n^-(x))^{m/2}\, d^m x \tag{123a}$$

and

$$\underline{\lim_{\lambda\to\infty}}\, N(\lambda)/\lambda^{m/2} \geq \tau_m(2\pi)^{-m} \int_{\{x \mid V_n^+(x)\leq 0\}} (-V_n^+(x))^{m/2}\, d^m x \tag{123b}$$

Since

$$\lim_{n\to\infty} \int_{\{x \mid V_n^\pm(x)\leq 0\}} (-V_n^\pm(x))^{m/2}\, d^m x = \int_{\{x \mid V(x)\leq 0\}} (-V(x))^{m/2}\, d^m x$$

on account of the continuity of V, (123) implies the theorem.

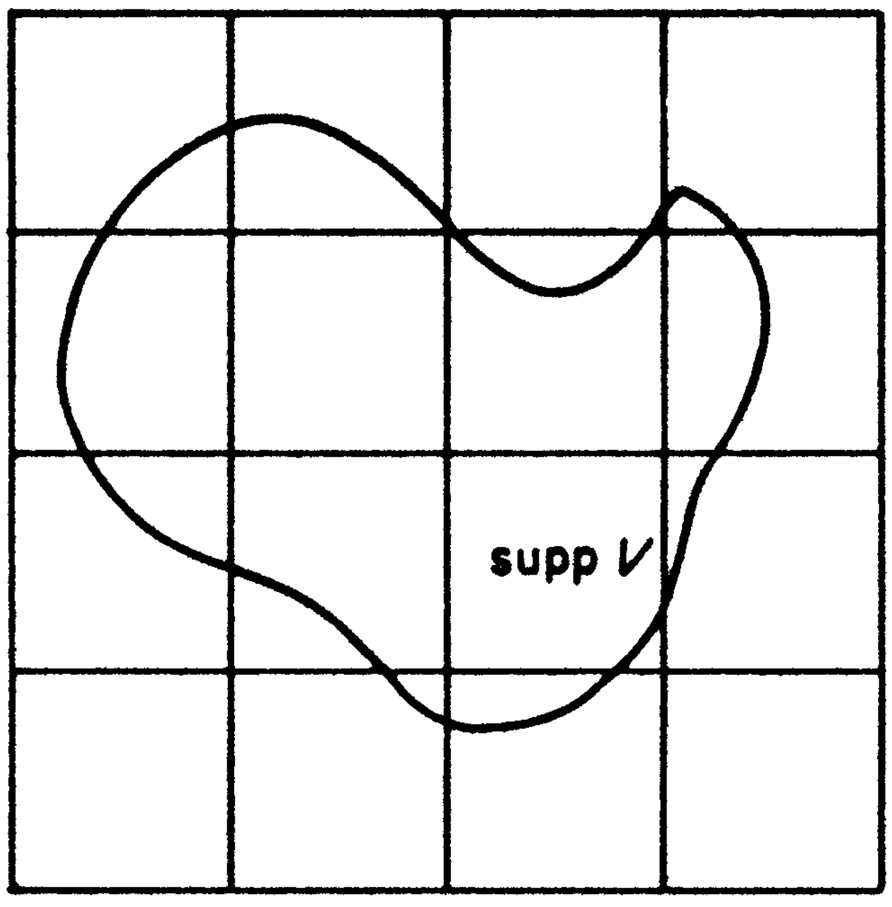


FIGURE XIII.12

Suppose that supp V is in a cube $(-k, k)^m$ with k integral. Let $-\Delta_+^n$ (respectively, $-\Delta_-^n$) be the Laplacian on all of $\mathbb{R}^m$ but with Dirichlet (respectively, Neumann) boundary conditions on the boundaries of all the 2^{-n} cubes in $(-k, k)^m$ (Figure XIII.12). Now, since $V_n^- \leq V \leq V_n^+$ and $-\Delta_-^n \leq -\Delta \leq -\Delta_+^n$, by Proposition 4, we have that

$$-\Delta_-^n + V_n^- \leq -\Delta + V \leq -\Delta_+^n + V_n^+$$

so with the obvious meaning for $N_n^\pm(\lambda)$, to prove (123) we need only prove that

$$\lim_{\lambda\to\infty} N_n^\pm(\lambda)/\lambda^{m/2} = \tau_m(2\pi)^{-m} \int_{V_n^\pm(x)\leq 0} (-V_n^\pm(x))^{m/2}\, dx \tag{124}$$

But, by the decoupling of Neumann and Dirichlet boundaries, $-\Delta_{\pm}^{n} + \lambda V_n^{\pm}$ is a direct sum of operators of the form $-\Delta_D^{\Omega} + \lambda c$ or $-\Delta_N^{\Omega} + \lambda c$ for constants c and cubes Ω and one positive operator given by the Laplacian on $\mathbb{R}^m \backslash (-k, k)^m$. Since for any positive operator A,

$$\dim((\text{Ran } P_{(-\infty, 0)}(A + \lambda c)) = \dim(\text{Ran } P_{[0, -\lambda c)}(A))$$

(124) follows from Proposition 2. ∎

The method of proof used to demonstrate the limit theorems does not extend to V's that are not at least locally bounded. However, one can extend the limit theorems by approximating nonsmooth V's by V's in C_0^∞. The critical element in this approximation argument is the existence of bounds on $N(V)$ that have the right coupling constant behavior, such as the Cwikel–Lieb–Rosenbljum bound (Theorem XIII.12).

Theorem XIII.80 For any $V \in L^{m/2}(\mathbb{R}^m)$, $m \geq 3$, one has

$$\lim_{\lambda \to \infty} N(\lambda V)/\lambda^{m/2} = \tau_m (2\pi)^{-m/2} \int_{V \leq 0} (-V(x))^{m/2}\, d^m x$$

Proof Let A be an arbitrary self-adjoint operator and let $\tilde{N}(A) = \dim(E_{(-\infty, 0)}(A))$ where $E_\Omega(A)$ is the spectral family for A. We first claim that

$$\tilde{N}(A + B) \leq \tilde{N}(A) + \tilde{N}(B) \tag{125}$$

for any self-adjoint operators A and B that are bounded below with $Q(A) \cap Q(B)$ dense and $A + B$ the form sum. (125) follows from the min–max principle: If $\tilde{N}(A), \tilde{N}(B) < \infty$, let $\psi_1, \ldots, \psi_{\tilde{N}(A)}$ be a basis for $E_{(-\infty, 0)}(A)$ and $\psi_{\tilde{N}(A)+1}, \ldots, \psi_{\tilde{N}(A)+\tilde{N}(B)}$ a basis for $E_{(-\infty, 0)}(B)$. If $\varphi \in Q(A) \cap Q(B)$ is in $[\psi_1, \ldots, \psi_{\tilde{N}(A)+\tilde{N}(B)}]^\perp$, then $(\varphi, A\varphi) \geq 0$ and $(\varphi, B\varphi) \geq 0$, so $\mu_{\tilde{N}(A)+\tilde{N}(B)+1}(A + B) \geq 0$ by the min–max principle. This proves (125).

Fix $\varepsilon > 0$, small. Choose $V_k \in C_0^\infty$ so that $V_k \to V$ in $L^{m/2}(\mathbb{R}^m)$. Then

$$-\Delta + \lambda V = [-(1 - \varepsilon)\Delta + \lambda V_k] + [\varepsilon(-\Delta) + \lambda(V - V_k)]$$

so that by (125) and $\tilde{N}(-\alpha\Delta + V) = N(\alpha^{-1} V)$,

$$\begin{aligned} N(\lambda V) &\leq N((1 - \varepsilon)^{-1} \lambda V_k) + N(\varepsilon^{-1} \lambda (V - V_k)) \\ &\leq N((1 - \varepsilon)^{-1} \lambda V_k) + c\varepsilon^{-m/2} \lambda^{m/2} \| V - V_k \|_{m/2}^{m/2} \end{aligned}$$

using (10). By the limit theorem just proven for $V_k \in C_0^\infty$,

$$\overline{\lim_{\lambda\to\infty}}\, N(\lambda V)/\lambda^{m/2} \leq (1-\varepsilon)^{-m/2}(2\pi)^{-m/2}\tau_m \int_{V_k\leq 0} (-V_k)^{m/2}\, d^m x + c\varepsilon^{-m/2}\|V - V_k\|_{m/2}^{m/2}$$

Taking $k\to\infty$ and then $\varepsilon\to 0$, we find that

$$\overline{\lim_{\lambda\to\infty}}\, N(\lambda V)/\lambda^{m/2} \leq (2\pi)^{-m/2}\tau_m \int_{V\leq 0} (-V)^{m/2}\, d^m x \tag{126}$$

Similarly,

$$-\Delta + \lambda V_k = [-(1-\varepsilon)\Delta + \lambda V] + [\varepsilon(-\Delta) + \lambda(V_k - V)]$$

so using the limit theorem and (10) as above,

$$(2\pi)^{-m/2}\tau_m \int_{V_k\leq 0} (-V_k)^{m/2}\, d^m x \leq \left[\underline{\lim_{\lambda\to\infty}}\, N(\lambda V)/\lambda^{m/2}\right](1-\varepsilon)^{-m/2} + c\varepsilon^{-m/2}\|V - V_k\|_{m/2}^{m/2}$$

Again taking $k\to\infty$ and then $\varepsilon\to 0$, we obtain

$$(2\pi)^{-m/2}\tau_m \int_{V\leq 0} (-V)^{m/2}\, d^m x \leq \underline{\lim_{\lambda\to\infty}}\, N(\lambda V)/\lambda^{m/2} \tag{127}$$

(126) and (127) imply the theorem. ∎

In our next result, which answers a question raised in Section 14, we make stronger assumptions on V than are absolutely necessary.

Theorem XIII.81 Let V be a measurable function on $\mathbb{R}^m$ ($m \geq 2$) obeying

$$c_1(|x|^\beta - 1) \leq V(x) \leq c_2(|x|^\beta + 1) \tag{128}$$

$$|V(x) - V(y)| \leq c_3[\max\{|x|, |y|\}]^{\beta-1}|x-y| \tag{129}$$

for some $\beta > 1$ and suitable constants c_1, c_2, $c_3 > 0$. Let $N(E) = \dim \operatorname{Ran} P_{(-\infty, E)}$ for $-\Delta + V$ and let

$$g(E) = \frac{\tau_m}{(2\pi)^m}\int_{\{x|V(x)\leq E\}} (E - V(x))^{m/2}\, d^m x \tag{130}$$

Then

$$\lim_{E\to\infty} N(E)/g(E) = 1$$

Proof Let $\{\Omega_\alpha\}$ be a list of all unit cubes with vertices at integral lattice points. Let V^+ (respectively, V^-) be that piecewise constant function with value $\sup_{\Omega_\alpha} V(x)$ (respectively, $\inf_{\Omega_\alpha} V(x)$) in the cube Ω_α. Let $-\Delta^+$ (respectively, $-\Delta^-$) be the Laplacian with Dirichlet (respectively, Neumann) boundary conditions on the sides of the cubes Ω_α. Let $N_\pm(E)$ be dim Ran $P_{(-\infty, E)}$ for $-\Delta^\pm + V^\pm$ and let $g_\pm(E)$ be given by (130) with V replaced by $V^\pm$. Then, by Dirichlet–Neumann bracketing,

$$N_-(E) \geq N(E) \geq N_+(E) \tag{131}$$

By (128) it is easy to see that

$$c_3(E^\gamma - 1) \leq g_+(E) \leq g(E) \leq g_-(E) \leq c_4(E^\gamma + 1) \tag{132}$$

where $\gamma = \frac{1}{2}m + m\beta^{-1}$. Moreover, by (129) and the bound

$$|(E-a)^{m/2} - (E-b)^{m/2}| \leq \frac{m}{2}\max[(E-a)^{\frac{1}{2}m-1}, (E-b)^{\frac{1}{2}m-1}]|b-a|$$

we have that

$$|g_-(E) - g_+(E)| \leq c_5(E^{\gamma-\beta^{-1}} + 1) \tag{133}$$

By (131)–(133), the theorem follows if we can prove that

$$\lim_{E\to\infty} N_\pm(E)/g_\pm(E) = 1 \tag{134}$$

By the decoupling nature of Dirichlet and Neumann boundary conditions

$$N_\pm(E) = \sum_{\{\alpha | V_\pm \restriction \Omega_\alpha \leq E\}} \eta_\pm(E - V_\pm \restriction \Omega_\alpha)$$

where $\eta_+(\lambda)$ (respectively, $\eta_-(\lambda)$) is dim(Ran $P_{[0,\lambda)}$) for $-\Delta$ in the unit cube with Dirichlet (respectively, Neumann) boundary conditions. By Proposition 2,

$$\left|\eta_\pm(\lambda) - \frac{\tau_m}{(2\pi)^m}\lambda^{m/2}\right| \leq c_6(1 + \lambda^{(m-1)/2})$$

Since

$$\sum_{\{\alpha | V_\pm \restriction \Omega_\alpha \leq E\}} \frac{\tau_m}{(2\pi)^m}(E - V_\pm \restriction \Omega_\alpha)^{m/2} = g_\pm(E)$$

we need only show that the error term

$$\varepsilon_\pm(E) \equiv \sum_{\{\alpha | V_\pm \restriction \Omega_\alpha \leq E\}} [1 + (E - V_\pm \restriction \Omega_\alpha)^{(m-1)/2}]$$

is small compared to $g_\pm(E)$. But clearly

$$\varepsilon_\pm(E) \leq (1 + E^{(m-1)/2}) \operatorname{vol}\{x \mid V_\pm(x) \leq E\}$$

By (128), this volume is bounded by const$(1 + E^{1/\beta})^m$ so

$$\varepsilon_\pm(E) \leq c_6(1 + E^{\gamma - \frac{1}{2}})$$

and therefore by (132),

$$\varepsilon_\pm(E)/g_\pm(E) \to 0$$

This proves (134) and thus completes the proof of the theorem. ∎

With some simple modifications, the theorem and proof extend to the case $m = 1$.

By methods similar to the above, one may prove the following result (Problem 131) which expresses how quickly dim Ran $P_{(-\infty, E]}$ diverges for those Schrödinger operators for which we proved dim Ran $P_{(-\infty, 0]} = \infty$ in Section 3.

Theorem XIII.82 Let V be a measurable function on $\mathbb{R}^m$ that obeys

$$-c_1(|x| + 1)^{-\beta} \leq V(x) \leq -c_2(|x| + 1)^{-\beta}$$

$$|V(x) - V(y)| \leq c_3[\min\{|x|, |y|\} + 1]^{-\beta - 1}|x - y|$$

for some $\beta < 2$ and $c_1, c_2, c_3 > 0$. Let $N(E) = \dim \operatorname{Ran} P_{(-\infty, -E]}$ for $-\Delta + V$ and let

$$g(E) = \frac{\tau_m}{(2\pi)^m} \int_{\{x \mid V(x) < -E\}} (-E - V(x))^{m/2}\, d^m x$$

Then

$$\lim_{E \downarrow 0} N(E)/g(E) = 1$$

We also note (Problem 132) that the asymptotic behavior of $N(E)$ is unchanged if we replace $-\Delta + V$ by $-\Delta + V + W$ where W is such that $-\Delta + \lambda W$ has only finitely many negative bound states for any λ. For example, this holds if W is in C_0^∞ (Problem 20) or in $L^{m/2}$ with $m \geq 3$.

By using methods quite different from those discussed thus far in this section, one can sometimes obtain more detailed information on the asymptotics of eigenvalues. Typical of further developments is the following:

Theorem XIII.82.5 Let H_0 be the operator $-d^2/dx^2$ on $L^2(0, 1)$ with the boundary conditions $u(0) = u(1) = 0$. Let $E_n(V)$ be the nth eigenvalue of $H_0 + V$. Then, for $V \in L^\infty(0, 1)$:

$$\lim_{n\to\infty} \left\{ E_n(V) - (n\pi)^2 - \int_0^1 V(x)\, dx \right\} = 0$$

Proof Fix $V \in L^\infty$, let $E_n(a) = E_n(aV)$, and let $\psi_n(a)$ be the eigenvector for $H(a) \equiv H_0 + aV$ with eigenvalue $E_n(a)$. Since $H(a)$ has only simple eigenvalues, the functions $E_n(a)$ are real analytic by the results of Section XII.2 and, in particular, by the explicit formulas of Section XII.1,

$$\frac{dE_n}{da}(a) = (\psi_n(a), V\psi_n(a))$$

$$\frac{d^2E_n}{da^2}(a) = -(V\psi_n(a), R_n(a)V\psi_n(a))$$

where $R_n(a)$ is the operator $(I - P_n(a))(H(a) - E_n(a))^{-1}$ with P_n the projection onto ψ_n. From the first formula, $|E_n(1) - E_n(0)| \leq \|V\|_\infty$ and, in particular, since $E_n(0) = (n\pi)^2$, we have that

$$|E_n(a) - E_{n-1}(a)| \geq (2n-1)\pi^2 - 2\|V\|_\infty a$$

It follows that for some N_0, and all $a \in (0, 1)$

$$\begin{aligned} R_n(a) &= \max(|E_n(a) - E_{n-1}(a)|^{-1}, |E_n(a) - E_{n+1}(a)|^{-1}) \\ &\leq cn^{-1} \end{aligned}$$

for all $n \geq N_0$. Thus, for such a and n, $d^2E_n(a)/da^2 \leq c\|V\|_\infty^2 n^{-1}$ so, by Taylor's theorem with remainder,

$$\left| E_n(1) - (n\pi)^2 - \frac{dE_n}{da}(0) \right| \leq \tfrac{1}{2}c\|V\|_\infty^2 n^{-1}$$

Since $\psi_n(0) = \sqrt{2}\sin(n\pi x)$, we conclude that at $a = 0$, $dE_n/da = \tilde{V}(0) - \frac{1}{2}\tilde{V}(2n) - \frac{1}{2}\tilde{V}(-2n)$ where $\tilde{V}(m) = \int_0^1 e^{-im\pi x}V(x)\, dx$. By the Riemann–Lebesgue lemma, $\tilde{V}(m) \to 0$ as $m \to \infty$, so $dE_n/da \to \tilde{V}(0)$ as $n \to \infty$. ∎

Notice that the error $E_n(V) - (n\pi)^2 - \int_0^1 V(x)\,dx$ is the sum of two terms, one of which is $O(n^{-1})$ and the other of which is Re $\tilde{V}(2n)$. For smooth V's, this term is also at least $O(n^{-1})$ but, in general, $\sup_{n \geq m} \tilde{V}(2n)$ can go to zero arbitrarily slowly. The above results depend critically on the one-dimensional nature of the problem, for it is only in one dimension that the distance between eigenvalues of H_0 diverges as n goes to infinity.

XIII.16 Schrödinger operators with periodic potentials

In this section we study Schrödinger operators $-\Delta + V$ where V is a periodic function. That is, we assume that for some basis $\{\mathbf{a}_i\}_{i=1}^n \in \mathbb{R}^n$, V satisfies

$$V(\mathbf{x} + \mathbf{a}_i) = V(\mathbf{x}) \tag{135}$$

As we shall discuss, these operators are important in solid state physics.

We have already seen that the spectral properties of Schrödinger operators are highly dependent on the behavior of V at infinity. Basically, we have studied three distinct classes of Schrödinger operators. The class whose spectral properties were easiest to establish were those with $V(x) \to \infty$ as $x \to \infty$; this class had empty essential spectrum (Theorem XIII.16). The next simplest class consisted of the "one-body Schrödinger operators" where $V(x) \to 0$ as $x \to \infty$, at least in some "average sense" (such as $V(x) \in L^p(\mathbb{R}^n, dx)$ for some $p < \infty$); under fairly general hypotheses these operators have $\sigma_{\text{ess}} = [0, \infty)$ (see Theorem XIII.15) and empty singular continuous spectrum (Theorem XIII.33). The third class is made up of the "N-body Schrödinger operators" for which $V(x) \to 0$ as $x \to \infty$ in "most" directions (i.e., those directions in which all "coordinate" differences $|\mathbf{r}_i - \mathbf{r}_j| \to \infty$) but for which V did not have a limit in tubes about those spatial directions where $\mathbf{r}_i = \mathbf{r}_j$ (some i, j). These operators were much harder to analyze; we saw that under fairly general circumstances $\sigma_{\text{ess}} = [\Sigma, \infty)$ where Σ was a "computable" number (Theorem XIII.17) but were only able to prove $\sigma_{\text{sing}} = \varnothing$ under specialized hypotheses (Theorems XIII.27, XIII.29, and XIII.36). We see therefore that spectral properties are very sensitive to the behavior of V at infinity. Since V's obeying (135) do not have a limit as $x \to \infty$ in any direction one might expect the analysis of periodic Schrödinger operators to be difficult.

The property that allows one to analyze $H = -\Delta + V$ when V is periodic is that H has a large symmetry group. For letting

$$(U(\mathbf{t})\psi)(\mathbf{x}) = \psi(\mathbf{x} + \sum_{i=1}^{n} t_i \mathbf{a}_i)$$

where $t \in \mathbb{Z}^n$, we see that (formally)

$$U(t)H = HU(t) \tag{136}$$

One can in fact prove that $U(t)e^{-iHs} = e^{-iHs}U(t)$ (Problem 135). A part of the analysis of H is then a special case of general symmetry arguments which are the subject of Chapter XVI. In this sense our discussion here is premature. We emphasize to the reader that the constant fiber direct integrals described below are an example of a construction from Chapter XVI (with most of the essential features) and that the fact that periodic Schrödinger operators have a direct integral decomposition is a direct consequence of (136). We remark that historically the essentials of the decomposition were discovered both by mathematicians (Floquet) and physicists (Bloch) who did not realize they were speaking group theory. We too shall not explicitly use the connection with the symmetry group here but will develop the theory directly.

Let $\mathscr{H}'$ be a separable Hilbert space and $\langle M, \mu \rangle$ a σ-finite measure space. In Section II.1, we constructed the Hilbert space $L^2(M, d\mu; \mathscr{H}')$ of square integrable $\mathscr{H}'$-valued functions. Notice that if μ is a sum of point measures at a finite set of points $m_1, \ldots, m_k$, then any $f \in L^2(M, d\mu; \mathscr{H}')$ is determined by the k-tuple $\langle f(m_1), \ldots, f(m_k) \rangle$ so $L^2(M, d\mu; \mathscr{H}')$ is isomorphic to the direct sum $\bigoplus_{i=1}^{m} \mathscr{H}'$. In some sense then, $L^2(M, d\mu; \mathscr{H}')$ for more general μ is a kind of "continuous direct sum" but with identical summands. We shall thus call $\mathscr{H} \equiv L^2(M, d\mu; \mathscr{H}')$ a **constant fiber direct integral** and write

$$\mathscr{H} = \int_M^{\oplus} \mathscr{H}' \, d\mu$$

It may seem silly to give an old familiar object a strange new name, but the new name is intended to convey a new emphasis on the "fibers" $\mathscr{H}'$ rather than the points of M. A particular class of operators on $\mathscr{H}$ will concern us. A function $A(\cdot)$ from M to $\mathscr{L}(\mathscr{H}')$ is called measurable if and only if for each $\varphi, \psi \in \mathscr{H}'$, $(\varphi, A(\cdot)\psi)$ is measurable. $L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$ denotes the space of (equivalence class of a.e. equal) measurable functions from M to $\mathscr{L}(\mathscr{H}')$ with

$$\|A\|_\infty \equiv \operatorname{ess\,sup} \|A(m)\|_{\mathscr{L}(\mathscr{H}')} < \infty$$

Definition A bounded operator A on $\mathscr{H} = \int_M^{\oplus} \mathscr{H}' \, d\mu$ is said to be **decomposed** by the direct integral decomposition if and only if there is a function $A(\cdot)$ in $L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$ so that for all $\psi \in \mathscr{H}$,

$$(A\psi)(m) = A(m)\psi(m) \tag{137}$$

We then call A **decomposable** and write

$$A = \int_M^{\oplus} A(m) \, d\mu(m)$$

The $A(m)$ are called the **fibers** of A.

We first note that every $A(\cdot)$ in $L^\infty(M, d\mu; \mathscr{H}')$ is associated with some decomposable operator:

Theorem XIII.83 If $A(\cdot) \in L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$, then there is a unique decomposable operator $A \in \mathscr{L}(\mathscr{H})$ so that (137) holds. Moreover $\|A\|_{\mathscr{L}(\mathscr{H})} = \|A(\cdot)\|_\infty$.

Proof Uniqueness is obvious. We must only show that (137) takes measurable square integrable $\mathscr{H}'$-valued functions ψ into measurable square integrable $\mathscr{H}'$-valued functions and that the operator A so defined is bounded with norm $\|A(\cdot)\|_\infty$. Let $\psi \in L^2(M, d\mu; \mathscr{H}')$. Let $\{\eta_k\}_{k=1}^\infty$ be an orthonormal basis for $\mathscr{H}'$. Then $A(m)\psi(m) = \sum_{k=1}^\infty (\eta_k, \psi(m))A(m)\eta_k$, a.e. in m since $A(\cdot)$ is a.e. a bounded operator. Now, by definition of measurability for $A(\cdot)$, $A(m)\eta_k$ is weakly measurable, so for any $N < \infty$, $\varphi_N(m) \equiv \sum_{k=1}^N (\eta_k, \psi(m))A(m)\eta_k$ is strongly measurable (Theorem IV.22). Moreover,

$$\begin{aligned}
\int \|\varphi_N(m)\|^2 \, d\mu &= \int \left\| A(m) \sum_{k=1}^N (\eta_k, \psi(m))\eta_k \right\|^2 d\mu \\
&\leq \|A(\cdot)\|_\infty^2 \int \left\| \sum_{k=1}^N (\eta_k, \psi(m))\eta_k \right\|^2 d\mu \\
&\leq \|A(\cdot)\|_\infty^2 \|\psi\|^2
\end{aligned} \tag{138}$$

A similar computation shows that that φ_N is Cauchy in $\mathscr{H}$. Thus it has a limit $\varphi \in L^2(M, d\mu; \mathscr{H}')$. But for almost all $m \in M$, $\varphi_N(m)$ converges to $A(m)\psi(m)$ in $\mathscr{H}'$. It follows that $A(\cdot)\psi(\cdot) \in L^2(M, d\mu; \mathscr{H}')$. By (138)

$$\|A(\cdot)\psi(\cdot)\| \leq \|A\|_\infty \|\psi\|$$

so A is bounded and $\|A\|_{\mathscr{L}(\mathscr{H})} \leq \|A(\cdot)\|_\infty$.

To prove the converse inequality, let $\{\beta_k\}_{k=1}^{\infty}$ be a dense subset of the unit ball in $\mathscr{H}'$ and let $f \in L^1(M, d\mu)$. We may decompose f as $f = gh$, with $g, h \in L^2$ and $\|g\|_2^2 = \|h\|_2^2 = \|f\|_1$. Fix k, ℓ and let $\psi = \bar{g}\beta_k$ and $\varphi = h\beta_\ell$. Then

$$\left| \int f(m)(\beta_k, A(m)\beta_\ell)\, d\mu \right| = |(\psi, A\varphi)| \leq \|A\| \, \|\psi\| \, \|\varphi\|$$

$$= \|A\| \, \|\beta_k\| \, \|\beta_\ell\| \int |f(m)|\, d\mu$$

Since $L^\infty(M)$ is the dual of $L^1(M)$, it follows that

$$|(\beta_k, A(m)\beta_\ell)| \leq \|\beta_k\| \, \|\beta_\ell\| \, \|A\|_{\mathscr{L}(\mathscr{H})}$$

a.e. in m. It follows that $\|A(\cdot)\|_\infty \leq \|A\|_{\mathscr{L}(\mathscr{H})}$. ∎

The above theorem sets up an isometric isomorphism of $L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$ and the decomposable operators on $\int_M^\oplus \mathscr{H}'\, d\mu$. Both these spaces are algebras in a natural way, and it is easy to see that the algebraic structure is preserved. $L^\infty(M, d\mu; \mathbb{C})$ is the natural subalgebra of $L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}'))$ corresponding to those decomposable operators whose fibers are all multiples of the identity.

Theorem XIII.84 Let $\mathscr{H} = \int_M^\oplus \mathscr{H}'\, d\mu$ where $\langle M, \mu \rangle$ is a separable σ-finite measure space and $\mathscr{H}'$ is separable. Let $\mathscr{A}$ be the algebra of decomposable operators whose fibers are all multiples of the identity. Then $A \in \mathscr{L}(\mathscr{H})$ is decomposable if and only if A commutes with each operator in $\mathscr{A}$.

Proof It is obvious that any decomposable A commutes with all the operators in $\mathscr{A}$, so we need only prove the converse. Since μ is σ-finite, we can find a strictly positive $F \in L^1$ so that $d\nu = F\, d\mu$ has unit mass. Let $\tilde{\mathscr{H}} = \int_M^\oplus \mathscr{H}'\, d\nu$. Then the map $U: \mathscr{H} \to \tilde{\mathscr{H}}$ by $Ug = F^{-1/2}g$ is unitary and $U\mathscr{A}U^{-1} = \tilde{\mathscr{A}}$. Moreover, A is decomposable if and only if UAU^{-1} is decomposable. As a result, we suppose without loss that $\int d\mu = 1$.

Suppose that A in $\mathscr{L}(\mathscr{H})$ commutes with any operator in $\mathscr{A}$. Choose an orthonormal basis $\{\eta_k\}_{k=1}^{\infty}$ for $\mathscr{H}'$ and let F_k be the element of $\mathscr{H}$ with $F_k(x) = \eta_k$ for all x. The F_k are orthonormal since $\int d\mu = 1$. Moreover, any $\psi \in \mathscr{H}$ has an expansion $\psi = \sum_{k=1}^{\infty} f_k(x)F_k$ with each $f_k \in L^2(M, d\mu; \mathbb{C})$ and $\|\psi\|^2 = \sum_k \|f_k\|^2$ (see Problem 12 of Chapter II). Define functions $a_{km}(x)$ by $AF_k = \sum_{m=1}^{\infty} a_{km}(x)F_m$. Choose a countable dense set D in $\mathscr{H}'$ of vectors of

the form $\sum_{k=1}^{N} \alpha_k \eta_k = \varphi$ and set $A(x)\varphi = \sum_{k,m} \alpha_k a_{km}(x)\eta_m$. Then, for any $f \in L^\infty(M, d\mu; \mathbb{C})$,

$$A(f\varphi) = f(A\varphi) = \sum_{k}^{N} f\alpha_k AF_k$$

$$= \sum_{k,m} f\alpha_k a_{km}(\cdot)F_m$$

since $f\mathbb{1} \in \mathscr{A}$. Thus

$$\int |f(x)|^2 \sum_{m} \left| \sum_{k} \alpha_k a_{km}(x) \right|^2 d\mu(x) \leq \|A\|^2 \left(\int |f(x)|^2 \right) \sum_{k} |\alpha_k|^2$$

It follows that, for almost all x and all $\varphi \in D$,

$$\|A(x)\varphi\| \leq \|A\| \, \|\varphi\|$$

so $A(x)$ can be extended to an operator on $\mathscr{L}(\mathscr{H}')$ and $A(\cdot) \in L^\infty$. Let B be the corresponding decomposable operator. Let $\psi \in \mathscr{H}$ have the form $\psi = \sum_{k=1}^{N} f_k(x)F_k$ with each $f_k \in L^\infty$. Then

$$(A\psi)(x) = \sum_{k=1}^{N} f_k(x)(AF_k(x)) = \sum_{k=1}^{N} f_k(x)(A(x)\eta_k) = A(x) \sum_{k=1}^{N} f_k(x)\eta_k$$

$$= (B\psi)(x)$$

Since such ψ's are dense, $A = B$. ∎

The construction we use below depends basically on the fact that the $U(t)$ generate an algebra that is isomorphic to the algebra $\mathscr{A}$ for a suitable constant fiber direct integral decomposition of $\mathscr{H} = L^2(\mathbb{R}^n, dx)$.

Since $-\Delta + V$ is unbounded, we need to discuss unbounded decomposable self-adjoint operators.

Definition A function $A(\cdot)$ from a measure space M to the (not necessarily bounded) self-adjoint operators on a Hilbert space $\mathscr{H}'$ is called **measurable** if and only if the function $(A(\cdot) + i)^{-1}$ is measurable. Given such a function, we define an operator A on $\mathscr{H} = \int_M^\oplus \mathscr{H}'$ with domain

$$D(A) = \left\{ \psi \in \mathscr{H} \;\middle|\; \psi(m) \in D(A(m)) \text{ a.e.}; \int_M \|A(m)\psi(m)\|_{\mathscr{H}'}^2 \, d\mu(m) < \infty \right\}$$

by

$$(A\psi)(m) = A(m)\psi(m)$$

We write $A = \int_M^\oplus A(m) \, d\mu$.

The properties of such operators are summarized by:

Theorem XIII.85 Let $A = \int_M^\oplus A(m)\, d\mu$ where $A(\cdot)$ is measurable and $A(m)$ is self-adjoint for each m. Then:

(a) The operator A is self-adjoint.
(b) A self-adjoint operator A on $\mathscr{H}$ has the form $\int_M^\oplus A(m)\, d\mu$ if and only if $(A + i)^{-1}$ is a bounded decomposable operator.
(c) For any bounded Borel function F on $\mathbb{R}$,

$$F(A) = \int_M^\oplus F(A(m))\, d\mu \tag{139}$$

(d) $\lambda \in \sigma(A)$ if and only if for all $\varepsilon > 0$,

$$\mu(\{m \mid \sigma(A(m)) \cap (\lambda - \varepsilon, \lambda + \varepsilon) \neq \varnothing\}) > 0$$

(e) λ is an eigenvalue of A if and only if

$$\mu(\{m \mid \lambda \text{ is an eigenvalue of } A(m)\}) > 0$$

(f) If each $A(m)$ has purely absolutely continuous spectrum, then so does A.
(g) Suppose that $B = \int_M^\oplus B(m)\, d\mu(m)$ with each $B(m)$ self-adjoint. If B is A-bounded with A-bound a, then a.e. $B(m)$ is $A(m)$-bounded with $A(m)$-bound $a(m) \leq a$. If $a < 1$, then

$$A + B = \int_M^\oplus (A(m) + B(m))\, d\mu \tag{140}$$

is self-adjoint on $D(A)$.

Proof (a) We first note that A is symmetric, so by the fundamental criterion, we need only prove that $\operatorname{Ran}(A \pm i) = \mathscr{H}$. Let $C(m) = (A(m) + i)^{-1}$. By hypothesis, $C(m)$ is measurable and $\|C(m)\| \leq 1$, so we can define $C = \int_M^\oplus C(m)\, d\mu$. Let $\psi = C\eta$ for $\eta \in \mathscr{H}$. Then, a.e., $\psi(m) \in \operatorname{Ran} C(m) = D(A(m))$ and

$$\|A(m)\psi(m)\| = \|A(m)C(m)\eta(m)\| \leq \|\eta(m)\| \in L^2(d\mu)$$

so $\psi \in D(A)$. Moreover $(A + i)\psi = \eta$ so $\operatorname{Ran}(A + i) = \mathscr{H}$. Similarly, since $(A(m) - i)^{-1} = C(m)^*$ is weakly measurable, $\operatorname{Ran}(A - i) = \mathscr{H}$.

(b) We leave this to the reader (Problem 136).

(c) Let us sketch the argument leaving the details to the reader (Problem 136). By the argument in (a), for any λ with $\operatorname{Im} \lambda \neq 0$,

$$(A - \lambda)^{-1} = \int_M^{\oplus} (A(m) - \lambda)^{-1} \, d\mu(m)$$

Since $e^{iAt} = \lim_{n \to \infty} (1 - (itA/n))^{-n}$ (by the functional calculus), one sees, employing the dominated convergence theorem, that

$$e^{iAt} = \int_M^{\oplus} e^{itA(m)} \, d\mu$$

If $F \in \mathscr{S}(\mathbb{R})$, (139) follows by use of the Fourier transform. By a suitable limiting argument, (139) holds for arbitrary F.

(d) A particular case of (139) is

$$P_{(a,b)}(A) = \int_M^{\oplus} P_{(a,b)}(A(m)) \, d\mu$$

Now (d) follows by noting that $\lambda \in \sigma(A)$ if and only if $P_{(\lambda-\varepsilon, \lambda+\varepsilon)}(A) \neq 0$ for all $\varepsilon > 0$ and that $\int_M^{\oplus} T(m) \, d\mu = 0$ if and only if $T(m) = 0$ a.e.

(e) The proof is similar to (d) using

$$P_{\{\lambda\}}(A) = \int_M^{\oplus} P_{\{\lambda\}}(A(m)) \, d\mu$$

(f) Let $\psi \in \mathscr{H}$ and let dv be the spectral measure for A associated to ψ. Let dv_m be the spectral measure for $A(m)$ associated to $\psi(m)$. Then

$$dv = \int_M (dv_m) \, d\mu(m)$$

in the sense that

$$\int_{\mathbb{R}} F(x) \, dv = \int_M \left(\int_{\mathbb{R}} F(x) \, dv_m \right) d\mu(m) \tag{141}$$

(141) follows immediately from (139). Now, if each $A(m)$ has purely absolutely continuous spectrum, then

$$dv_m(x) = g_m(x) \, dx$$

for some $g_m \in L^1(\mathbb{R}, dx)$ with $\int g_m(x) \, dx = \|\psi(m)\|_{\mathscr{H}}^2$. Thus

$$g(x) = \int g_m(x) \, d\mu(m)$$

is in $L^1(\mathbb{R}, dx)$ and, by (141),

$$dv = g(x)\,dx$$

It follows that $\psi \in \mathscr{H}_{\mathbf{ac}}$ for A, so that A has purely absolutely continuous spectrum.

(g) If $\|B\psi\| \leq a\|A\psi\| + b\|\psi\|$, then $\|B(A + ik)^{-1}\| \leq a + bk^{-1}$ for any positive integer k. Therefore,

$$\|B(m)(A(m) + ik)^{-1}\| \leq a + bk^{-1}$$

a.e. so $B(m)$ is $A(m)$-bounded with bound $a(m) \leq a$. (140) is immediate. ∎

Part (f) of this last theorem says that a sufficient condition for $A = \int_M^{\oplus} A(m)\,d\mu(m)$ to have purely absolutely continuous spectrum is that each $A(m)$ have purely absolutely continuous spectrum. But this is certainly not necessary. In fact, A can have purely absolutely continuous spectrum even though each $A(m)$ has purely discrete spectrum! The following theorem illustrates the phenomenon.

Theorem XIII.86 Let $\langle M, d\mu\rangle$ be $[0, 1]$ with Lebesgue measure. Let $\mathscr{H}'$ be a fixed separable infinite-dimensional space and let $A = \int_{[0,1]}^{\oplus} A(m)\,d\mu(m)$ with each $A(m)$ self-adjoint. Suppose we are given $\mathscr{H}'$-valued functions $\{\psi_n(\cdot)\}_{n=1}^{\infty}$ on $[0, 1]$, real analytic on $(0, 1)$, continuous on $[0, 1]$, and complex-valued functions $E_n(\cdot)$, analytic in a neighborhood of $[0, 1]$, so that:

(i) No $E_n(\cdot)$ is constant.

(ii) $A(m)\psi_n(m) = E_n(m)\psi_n(m)$ for all $m \in [0, 1]$; $n = 1, 2, \ldots$.

(iii) For each m, the set $\{\psi_n(m)\}_{n=1}^{\infty}$ is a complete orthonormal basis for $\mathscr{H}'$.

Then A has purely absolutely continuous spectrum.

Proof Let

$$\mathscr{H}_n = \{\psi \in \mathscr{H} \mid \psi(m) = f(m)\psi_n(m); f \in L^2(M; d\mu)\}$$

Then the $\mathscr{H}_n$ are closed subspaces that are mutually orthogonal and $\mathscr{H} = \bigoplus \mathscr{H}_n$ since any $\psi \in \mathscr{H}$ has an expansion (Problem 134):

$$\psi = \sum_{n=1}^{\infty} (\psi_n(m), \psi(m))\psi_n(m)$$

Moreover, each $\mathscr{H}_n$ lies in $D(A)$ with $A[\mathscr{H}_n] \subset \mathscr{H}_n$. Consider the unitary map U_n: $\mathscr{H}_n \to L^2([0, 1], dx)$, given by $U_n(f(m)\psi_n(m)) = f(m)$. Then $A_n \equiv U_n A U_n^{-1}$ is given by

$$(A_n f)(m) = E_n(m)f(m) \tag{142}$$

We need only show that each A_n has purely absolutely continuous spectrum. Since $E_n(\cdot)$ is analytic in a neighborhood of $[0, 1]$ and nonconstant, dE_n/dm has only finitely many zeros in $(0, 1)$, say at $m_1, \ldots, m_{k-1}$. Let $m_0 = 0$ and $m_k = 1$. Then

$$L^2([0, 1], dx) = \bigoplus_{j=1}^{k} L^2((m_{j-1}, m_j), dx)$$

A_n leaves each summand invariant and acts on the summand by (142). On each interval (m_{j-1}, m_j), $E_n(\cdot)$ is strictly monotone, either increasing or decreasing. Consider the case where it is increasing. Define α: $(E_n(m_{j-1}), E_n(m_j)) \to (m_{j-1}, m_j)$ by $E_n(\alpha(\lambda)) = \lambda$. Then α is differentiable and the Stieltjes measure $d\alpha$ is absolutely continuous with respect to dx. In fact,

$$d\alpha = \left[\left(\frac{dE}{dm}\right)\Big|_{m=\alpha(\lambda)}\right]^{-1} d\lambda$$

Let U be the unitary operator from $L^2((m_{j-1}, m_j), dx)$ to $L^2((E_n(m_{j-1}), E_n(m_j)), d\lambda)$ given by

$$(Uf)(\lambda) = \left(\frac{d\alpha}{d\lambda}\right)^{+1/2} f(\alpha(\lambda))$$

Then

$$(UA_nU^{-1})g(\lambda) = \lambda g(\lambda)$$

We have thus explicitly constructed a spectral representation for $A_n \restriction L^2([m_{j-1}, m_j], dx)$ for which the spectral measure $d\alpha$ is Lebesgue measure. It follows that each A_n, and thus A, has purely absolutely continuous spectrum. ∎

We turn now to an analysis of Schrödinger operators with periodic potentials. We first consider the case of one dimension with V piecewise continuous where differential equation methods are available and then the case of higher dimension and more general V.

To motivate our analysis, suppose that $V \in C_0^\infty(\mathbb{R})$ with bounded derivatives so that $-d^2/dx^2 + V$ takes $\mathscr{S}(\mathbb{R})$ into itself. If $f \in \mathscr{S}(\mathbb{R})$, then

$$\left[\left(-\frac{d^2}{dx^2} + V\right)f\right]\hat{}\,(p) = p^2\hat{f}(p) + (2\pi)^{-1/2}\int \hat{V}(p - p')\hat{f}(p')\,dp' \quad (143)$$

where the integral in (143) is a formal symbol for the convolution of the distribution $\hat{V}$ and the function $\hat{f}$. Now, let us suppose that V has period 2π. Then V has a uniformly convergent Fourier series (see Theorem II.8):

$$V(x) = \sum_{n=-\infty}^{\infty} \tilde{V}_n e^{inx} \tag{144}$$

where

$$\tilde{V}_n = \int_{-\pi}^{\pi} \tilde{V}(x) e^{-inx} \frac{dx}{2\pi}$$

(144) suggests that

$$(2\pi)^{-\frac{1}{2}} \hat{V}(p) = \sum_{n=-\infty}^{\infty} \tilde{V}_n \delta(p-n) \tag{145}$$

since putting (145) formally into the Fourier inversion formula yields (144). In fact, one can prove (145) as follows: If $f \in \mathscr{S}(\mathbb{R})$, then the uniform convergence of (144) implies that

$$\int f(x)V(x)\,dx = (2\pi)^{1/2} \sum_{n=-\infty}^{\infty} \tilde{V}_n \hat{f}(n)$$

from which (145) follows if the sum is viewed as convergent in the weak $(\sigma(\mathscr{S}', \mathscr{S}))$ topology on $\mathscr{S}'$.

Now that we have analyzed Fourier transforms of periodic tempered distributions, we can use this analysis to rewrite (143) as

$$\left[\left(-\frac{d^2}{dx^2} + V\right) f\right]\hat{}\,(p) = p^2 \hat{f}(p) + \sum_{n=-\infty}^{\infty} \tilde{V}_n \hat{f}(p-n)$$

Thus, if $H = -d^2/dx^2 + V$, then $\widehat{Hf}(p)$ depends only on the values $\hat{f}(p-n)$; $n \in \mathbb{Z}$. We have therefore proven:

Theorem XIII.87 (direct integral decomposition of periodic Schrödinger operators—p-space version in one dimension) Let $\mathscr{H}' = \ell_2$ and let $\mathscr{H} = \int_{(-1/2,\,1/2]}^{\oplus} \mathscr{H}'\,dx$. For $q \in (-\frac{1}{2}, \frac{1}{2}]$, let

$$(H(q)g)_j = (q+j)^2 g_j + \sum_{n=-\infty}^{\infty} \tilde{V}_n g_{j-n}$$

where $\tilde{V}_n$ are the Fourier series coefficients of some $V \in C^\infty(\mathbb{R})$ with period 2π. Map $L^2(\mathbb{R}, dx)$ to $\mathscr{H}$ by

$$[(Uf)(q)]_j = \hat{f}(q + j)$$

Let $H = -d^2/dx^2 + V$ on $L^2(\mathbb{R})$. Then,

$$UHU^{-1} = \int_{(-1/2,\, 1/2]}^{\oplus} H(q)\, dq$$

One can get quite far in the analysis of H by using this p-space version of the direct integral decomposition. In fact, this will be our main tool in the multidimensional case. However, in the one-dimensional case, the x-space translation of Theorem XIII.87 gives a little more information. While we could use Theorem XIII.87 directly to write down the x-space version, we shall give an independent proof, using Theorem XIII.87 merely for the following motivation. In case $V = 0$ the operator $H(q)$ has eigenvalues $(q + j)^2$ and eigenfunctions that are basically the Fourier transforms of the functions $e^{i(q+j)x}$. This suggests that somehow $H(q)$ is related to the operator $-d^2/dx^2$ on $L^2([0, 2\pi], dx)$ but with the boundary conditions

$$\psi(2\pi) = e^{2\pi i q}\psi(0), \qquad \psi'(2\pi) = e^{2\pi i q}\psi'(0)$$

Lemma Let $\mathscr{H}' = L^2([0, 2\pi], dx)$. Let

$$\mathscr{H} = \int_{[0,\, 2\pi)}^{\oplus} \mathscr{H}' \frac{d\theta}{2\pi} \tag{146}$$

Then $U: L^2(\mathbb{R}, dx) \to \mathscr{H}$ given by

$$(Uf)_\theta(x) = \sum_{n=-\infty}^{\infty} e^{-i\theta n} f(x + 2\pi n) \tag{147}$$

for θ and x in $[0, 2\pi)$, is well defined for $f \in \mathscr{S}(\mathbb{R})$ and uniquely extendable to a unitary operator. Moreover,

$$U\left(-\frac{d^2}{dx^2}\right)U^{-1} = \int_{[0,\, 2\pi)}^{\oplus} \left(-\frac{d^2}{dx^2}\right)_\theta \frac{d\theta}{2\pi} \tag{148}$$

where $(-d^2/dx^2)_\theta$ is the operator $-d^2/dx^2$ on $L^2([0, 2\pi])$ with the boundary conditions

$$\psi(2\pi) = e^{i\theta}\psi(0), \qquad \psi'(2\pi) = e^{i\theta}\psi'(0)$$

Proof For $f \in \mathscr{S}$, the sum (147) is clearly convergent. To prove that Uf is in $\mathscr{H}$, we compute that for $f \in \mathscr{S}$,

$$\int_0^{2\pi} \left(\int_0^{2\pi} \left| \sum_{n=-\infty}^{\infty} e^{-in\theta} f(x + 2\pi n) \right|^2 dx \right) \frac{d\theta}{2\pi}$$

$$= \int_0^{2\pi} \left[\left(\sum_{n=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \overline{f(x + 2\pi n)} f(x + 2\pi j) \right) \int_0^{2\pi} e^{-i(j-n)\theta} \frac{d\theta}{2\pi} \right] dx$$

$$= \int_0^{2\pi} \left(\sum_{n=-\infty}^{\infty} |f(x + 2\pi n)|^2 \right) dx = \int_{-\infty}^{\infty} |f(x)|^2 \, dx$$

where we have used the Fubini and Plancherel theorems. Thus we see that U is well defined and has a unique extension to an isometry. To see that U is onto $\mathscr{H}$, we compute U^*. For $g \in \mathscr{H}$, we define, for $0 \le x \le 2\pi$, $n \in \mathbb{Z}$,

$$(U^*g)(x + 2\pi n) = \int_0^{2\pi} e^{in\theta} g_\theta(x) \frac{d\theta}{2\pi} \tag{149}$$

A direct computation shows that this is indeed the formula for the adjoint of U. Moreover,

$$\|U^*g\|_2^2 = \int_{-\infty}^{\infty} |(U^*g)(y)|^2 \, dy$$

$$= \int_0^{2\pi} \left(\sum_{n=-\infty}^{\infty} |(U^*g)(2\pi n + x)|^2 \right) dx$$

$$= \int_0^{2\pi} \left(\sum_{n=-\infty}^{\infty} \left| \int e^{in\theta} g_\theta(x) \frac{d\theta}{2\pi} \right|^2 \right) dx$$

$$= \int_0^{2\pi} \left(\int_0^{2\pi} |g_\theta(x)|^2 \frac{d\theta}{2\pi} \right) dx$$

$$= \|g\|^2$$

In the next to the last step we have used the Parseval relation for Fourier series.

To verify (148), let A be the operator on the right-hand side of (148). We shall show that if $f \in \mathscr{S}(\mathbb{R})$, then $Uf \in D(A)$ and $U(-f'') = A(Uf)$. Since $-d^2/dx^2$ is essentially self-adjoint on $\mathscr{S}$ and A is self-adjoint, (148) will follow. So, suppose $f \in \mathscr{S}(\mathbb{R}^n)$. Then Uf is given by the convergent sum (147)

so that Uf is C^∞ on $(0, 2\pi)$ with $(Uf)'_\theta(x) = (Uf')_\theta(x)$ and similarly for higher derivatives. Moreover, it is clear that

$$(Uf)_\theta(2\pi) = \sum_{n=-\infty}^{\infty} e^{-i\theta n} f(2\pi(n+1))$$

$$= \sum_{n=-\infty}^{\infty} e^{-i\theta(n-1)} f(2\pi n) = e^{i\theta}(Uf)_\theta(0)$$

Similarly, $(Uf)'_\theta(2\pi) = e^{i\theta}(Uf_\theta)'(0)$. Thus, for each θ, $(Uf)_\theta \in D((-d^2/dx^2)_\theta)$ and

$$\left(-\frac{d^2}{dx^2}\right)_\theta (Uf) = U(-f'')_\theta$$

We conclude that $Uf \in D(A)$ and $A(Uf) = U(-f'')$. This proves (148). ∎

Theorem XIII.88 (direct integral decomposition of periodic Schrödinger operators—x-space version in one dimension) Let V be a bounded measurable function on $\mathbb{R}$ with period 2π. For $\theta \in [0, 2\pi)$, let

$$H(\theta) = \left(-\frac{d^2}{dx^2}\right)_\theta + V(x)$$

as an operator on $L^2[0, 2\pi]$. Let U be given by (147). Then, under the decomposition (146),

$$U\left(-\frac{d^2}{dx^2} + V\right)U^{-1} = \int_{[0, 2\pi)}^{\oplus} H(\theta)\frac{d\theta}{2\pi} \tag{150}$$

Proof Let V be the θ-independent operator acting on the fiber $\mathscr{H}' = L^2([0, 2\pi), dx)$ by

$$(V_\theta f)(x) = V(x)f(x), \qquad 0 \le x \le 2\pi$$

(150) follows from Theorem XIII.85g and the lemma if we can prove that

$$UVU^{-1} = \int_{[0, 2\pi)}^{\oplus} V_\theta \frac{d\theta}{2\pi} \tag{151}$$

By (147), for $f \in \mathscr{S}$,

$$(UVf)_\theta(x) = \sum_{n=-\infty}^{\infty} e^{-in\theta} V(x + 2\pi n) f(x + 2\pi n)$$

$$= V(x) \sum_{n=-\infty}^{\infty} e^{-in\theta} f(x + 2\pi n)$$

$$= V_\theta (Uf)_\theta(x)$$

since V is periodic. This proves (151) and so (150). ∎

As a result, to analyze $-d^2/dx^2 + V$ with V periodic, we need only analyze $(-d^2/dx^2)_\theta + V$ for each θ. As a preliminary, we note:

Lemma

(a) For each $\theta \in [0, 2\pi)$, $(-d^2/dx^2)_\theta$ has compact resolvent.
(b) For $\theta = 0$, $\exp(-t(-d^2/dx^2)_{\theta=0})$ is a positivity improving semigroup (see Section 12).
(c) $[(-d^2/dx^2)_\theta + 1]^{-1}$ is an analytic operator-valued function of θ in a neighborhood of $[0, 2\pi)$.

Proof We shall later prove the analogue of this lemma in the multi-dimensional case by using general arguments that could be used here. However, it is easy to obtain explicit formulas for $K_\theta \equiv [(-d^2/dx^2)_\theta + 1]^{-1}$. Let $f \in C_0^\infty(0, 2\pi)$. Let K be the inverse of $-d^2/dx^2 + 1$ defined on all of $L^2(\mathbb{R})$. Let $g = Kf$. By our arguments in Section IX.7, K is an integral operator with kernel $G(x - y)$ where $\hat{G}(p) = (2\pi)^{-1/2}(p^2 + 1)^{-1}$. A direct computation of G is possible (Problem 137) and one finds

$$g(x) \equiv Kf(x) = \tfrac{1}{2} \int e^{-|x-y|} f(y)\, dy \tag{152}$$

Now, both Kf and $K_\theta f$ solve the differential equation $-u''(x) + u(x) = f(x)$ on $(0, 2\pi)$. It follows that their difference $v = K_\theta f - Kf$ obeys $-v'' + v = 0$ so that

$$(K_\theta f)(x) = g(x) + ae^x + be^{-x}$$

Since $K_\theta f \in D((-d/dx^2)_\theta)$, a and b must be chosen so that $K_\theta f$ obeys the boundary conditions

$$u(2\pi) = e^{i\theta}u(0), \qquad u'(2\pi) = e^{i\theta}u'(0) \tag{153}$$

Direct computation using (152) shows that

$$(K_\theta f)(x) = \int_0^{2\pi} G_\theta(x, y) f(y)\, dy$$

$$G_\theta(x, y) = \tfrac{1}{2}e^{-|x-y|} + \alpha(\theta)e^{x-y} + \beta(\theta)e^{y-x} \tag{154}$$

$$\alpha(\theta) = \tfrac{1}{2}(e^{2\pi - i\theta} - 1)^{-1}$$

$$\beta(\theta) = \tfrac{1}{2}(e^{2\pi + i\theta} - 1)^{-1}$$

One can read the properties claimed for $(-d^2/dx^2)_\theta$ directly from (154). Since $G_\theta(x, y)$ is bounded in x, y for each fixed θ,

$$\int_0^{2\pi}\int_0^{2\pi} |G_\theta(x, y)|^2\, dx\, dy < \infty$$

so K_θ is Hilbert–Schmidt and so compact, proving (a). By direct examination, the kernel $G_{\theta=0}(x, y)$ is strictly positive. A similar computation proves that $[(-d^2/dx^2)_{\theta=0} + a]^{-1}$ has a strictly positive kernel for any $a > 0$ and so by Theorem XIII.44 and the preceding proposition, $\exp(-t(-d^2/dx^2)_{\theta=0})$ is a positivity improving semigroup. Finally, to prove (c), we note that the formulas (154) allow us to define a Hilbert–Schmidt operator K_θ for any θ with $|\operatorname{Im}\theta| < 2\pi$ and that $\theta \to K_\theta$ is clearly analytic in θ. ∎

It may seem striking at first sight that $K_\theta - K_{\theta'}$ is a rank two operator for any θ, θ', but, in fact, this is just a reflection of the fact that $-d^2/dx^2 \restriction C_0^\infty(0, 2\pi)$ has deficiency indices $\langle 2, 2\rangle$ so that K_θ is completely determined in a θ-independent way on the closure of the space $(-d^2/dx^2 + 1)[C_0^\infty(0, 2\pi)]$ which has codimension 2.

An analysis similar to that above shows that $((-d^2/dx^2)_\theta + a)^{-1}$ is analytic in the region $|\operatorname{Im}\theta| < 2\pi\sqrt{a}$ so that the map $\theta \mapsto (-d^2/dx^2)_\theta$ can be extended to an entire analytic family. This family is neither type (A) nor type (B).

Armed with the lemma, we are prepared for a complete analysis of the operators

$$H(\theta) = \left(-\frac{d^2}{dx^2}\right)_\theta + V \tag{155}$$

Theorem XIII.89 Suppose that V is piecewise continuous and periodic of period 2π. Then:

(a) $H(\theta)$ has purely discrete spectrum and is real analytic in θ.
(b) $H(\theta)$ and $H(2\pi - \theta)$ are antiunitarily equivalent under ordinary complex conjugation. In particular, their eigenvalues are identical and their eigenfunctions are complex conjugates.
(c) For $\theta \in (0, \pi)$, or in $(\pi, 2\pi)$, $H(\theta)$ has only nondegenerate eigenvalues.
(d) Let $E_n(\theta)$ $(n = 1, 2, \ldots; 0 \le \theta \le \pi)$ denote the nth eigenvalue of $H(\theta)$. Then each $E_n(\cdot)$ is analytic in $(0, \pi)$ and continuous at $\theta = 0$ and π.

(e) For n odd (respectively, even) $E_n(\theta)$ is strictly monotone increasing (respectively, decreasing) as θ increases from 0 to π. In particular,

$$E_1(0) < E_1(\pi) \leq E_2(\pi) < E_2(0) \leq \cdots \leq E_{2n-1}(0) < E_{2n-1}(\pi) \leq E_{2n}(\pi) < E_{2n}(0) \leq \cdots$$

See Figure XIII.13.

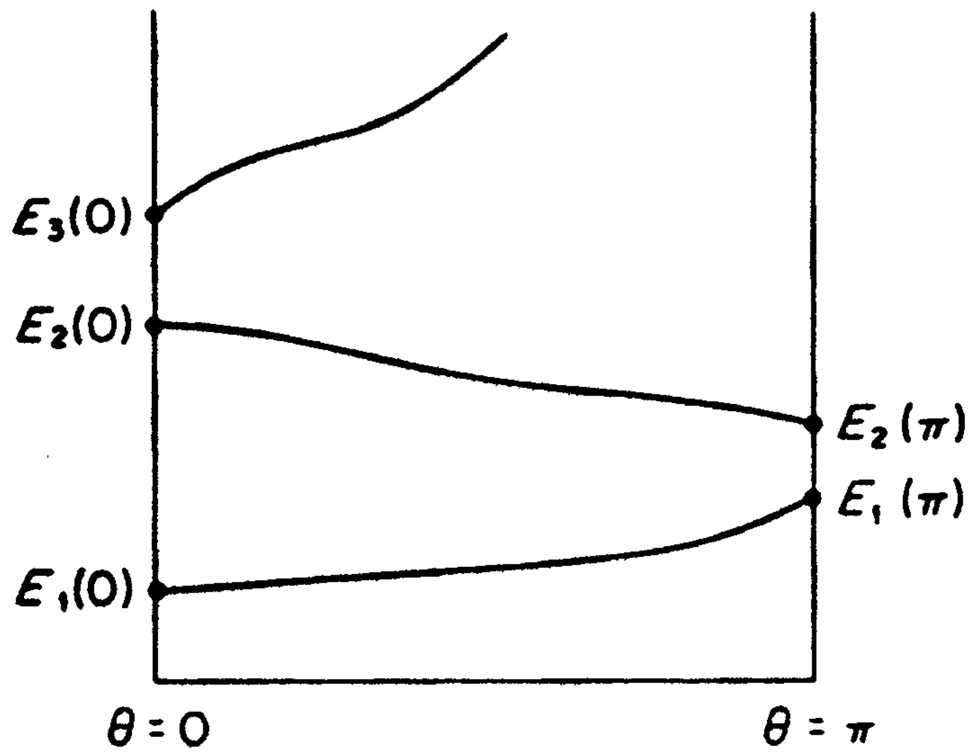


FIGURE XIII.13 Bands in one-dimensional Schrödinger operators.

(f) One can choose the eigenvectors $\psi_n(\theta)$ so that they are analytic in θ for $\theta \in (0, \pi) \cup (\pi, 2\pi)$, continuous at π and 0 (with $\psi_n(0) = \psi_n(2\pi)$).

Proof (a) This follows directly from the lemma and the basic perturbation Theorems XII.11 and XIII.64.

(b) When $V = 0$, this is a simple consequence of the definition of $(-d^2/dx^2)_\theta$. Since $\overline{V\psi} = V\overline{\psi}$, the results hold for general V.

(c) If E is an eigenvalue of $H(\theta)$, $\theta \in (0, \pi)$, then $-u'' + Vu = Eu$ has a solution obeying the boundary condition (153). So $\bar{u}$ is a solution obeying a distinct boundary condition. Since $-u'' + Vu = Eu$ has only two linearly independent solutions and not all of them obey (153), at most one can.

(d) Consider $E_1(0)$. This is a simple eigenvalue of $H(0)$ since $H(0)$ generates a positivity preserving semigroup. Since $H(\theta)$ is analytic near $\theta = 0$, we can find $\tilde{f}_1(\theta)$ an eigenvalue of $H(\theta)$ for $\theta \in [0, \varepsilon)$ analytic in $[0, \varepsilon)$ with $\tilde{f}_1(0) = E_1(0)$. Let $\varepsilon < \pi$. The only thing that can prevent one from analytically continuing past $\theta = \varepsilon$ is if $\tilde{f}_1(\theta) \to \infty$ as $\theta \uparrow \varepsilon$. For since $H(\theta) \geq -\|V\|_\infty$, if $\tilde{f}_1(\theta)$ does not approach ∞, then there is a sequence $\theta_n \to \varepsilon$ such that $\tilde{f}_1(\theta_n) \to \tilde{E}$. But then one sees that $\tilde{E}$ is an eigenvalue of $H(\varepsilon)$. By (c), it is a simple eigenvalue, so for $|\theta - \varepsilon| < \delta$, there is a unique eigenvalue $g(\theta)$ of $H(\theta)$ near $\tilde{E}$ and g is analytic for $|\theta - \varepsilon| < \delta$. In particular, for n large $g(\theta_n) = \tilde{f}_1(\theta_n)$ so g provides an analytic continuation for $\tilde{f}_1$ past ε. Thus to prove that $\tilde{f}_1$ can be analytically continued to all of $[0, \pi)$, we need only show that $\tilde{f}_1(\theta)$ remains finite as θ varies. We first show that $H(\theta)$

has no eigenvalue smaller than $\tilde{f}_1(\theta)$ if $\theta \in [0, \varepsilon)$. If it did, we could continue that back to $\theta = 0$; this continuation could not go to infinity as we decreased θ since it is always strictly less than $\tilde{f}_1(\theta)$ by the simplicity of eigenvalues and the argument above. Continuing back to $\theta = 0$, we would find an eigenvalue less than E_1. Since $\tilde{f}_1(\theta)$ is the smallest eigenvalue of $H(\theta)$ it cannot go to infinity as $\theta \to \varepsilon$. Thus, $\tilde{f}_1(\theta)$ has a continuation to $[0, \pi]$ and this continuation is the smallest eigenvalue of $H(\theta)$, i.e., it is $E_1(\theta)$.

Now look at $E_2(0)$. This may be doubly degenerate; for example it is when $V = 0$. If it is though, the degeneracy must be broken for $\theta \neq 0$ since the spectrum of $H(\theta)$, $\theta \neq 0$ is simple. By degenerate perturbation theory, the eigenvalue (or eigenvalues if $E_2(0)$ is degenerate) near $E_2(0)$ is given by analytic function(s). Let $\tilde{f}_2(\theta)$ be this function if $E_2(0)$ is simple, and the smaller of the functions if $E_2(0)$ is degenerate. Then by mimicking the argument above, $\tilde{f}_2(\theta)$ can be continued throughout $[0, \pi]$ and is the second eigenvalue $E_2(\theta)$. By repeating this argument, we can handle all the eigenvalues.

(e) This is the deepest part of the theorem, so we shall give a detailed proof. As a preliminary, we prove that $E_1(0) \leq E_1(\theta)$ for all θ. Since $e^{-tH(0)}$ is positivity improving, the eigenvector $\psi_1(0)$ associated to $E_1(0)$ is strictly positive and by the boundary condition, it has a periodic extension to all of $\mathbb{R}$. Fix k, an integer, and consider $H^{(k)}(0)$ the operator $-d^2/dx^2 + V$ on $L^2(-2\pi k, 2\pi k)$ with periodic boundary conditions. Then $\psi_1(0)$ periodically extended is a strictly positive eigenvector of $H^{(k)}(0)$ and so $E_1(0) = \inf \sigma(H^k(0))$ (see Section XIII.12). It follows that if $f \in C_0^\infty(-2\pi k, 2\pi k)$, then $(f, (-d^2/dx^2 + V)f) = (f, H^k(0)f) \geq E_1(f, f)$, and thus the operator $-d^2/dx^2 + V$ on $L^2(\mathbb{R})$ obeys $-d^2/dx^2 + V \geq E_1$. By the direct integral decomposition, $H(\theta) \geq E_1(0)$, a.e. in θ so $E_1(\theta) \geq E_1(0)$, a.e. in θ. Since $E_1(\theta)$ is continuous $E_1(\theta) \geq E_1(0)$ for all $\theta \in (0, 2\pi)$.

Now we introduce an important function, $D(E)$, associated to the differential equation

$$-u'' + Vu = Eu \tag{156}$$

Let $u_1(E, x)$ be the solution of (156) with $u_1(0) = 1$, $u_1'(0) = 0$, and let $u_2(E, x)$ be the solution of (156) with $u_2(0) = 0$, $u_2'(0) = 1$. Then $u_i(x, E)$ is analytic in E for each x by the standard theory of ordinary differential equations. Let $M(E)$ be the analytic two by two matrix

$$M(E) = \begin{bmatrix} u_1(E, 2\pi) & u_2(E, 2\pi) \\ u_1'(E, 2\pi) & u_2'(E, 2\pi) \end{bmatrix} \tag{157}$$

The **discriminant** of $-u'' + Vu$ is the function

$$D(E) \equiv \mathrm{Tr}(M(E)) = u_1(E, 2\pi) + u_2'(E, 2\pi)$$

$M(E)$ is a natural object, for if v satisfies (156), then

$$\begin{bmatrix} v(2\pi) \\ v'(2\pi) \end{bmatrix} = M(E) \begin{bmatrix} v(0) \\ v'(0) \end{bmatrix}$$

In particular, the equation $H(\theta)\psi = E\psi$ has a nonzero solution if and only if $M(E)$ has an eigenvalue $e^{i\theta}$. Now $M(E)$ has determinant 1 since $W(x) = u_1(E, x)u_2'(E, x) - u_1'(E, x)u_2(E, x)$ is a constant. Thus its eigenvalues are λ and λ^{-1} and $D(E) = \lambda + \lambda^{-1}$. We conclude that *$E$ is an eigenvalue of $H(\theta)$ if and only if $D(E) = 2 \cos \theta$*. What we will prove is that $D(E)$ has a graph somewhat like the one in Figure XIII.14.

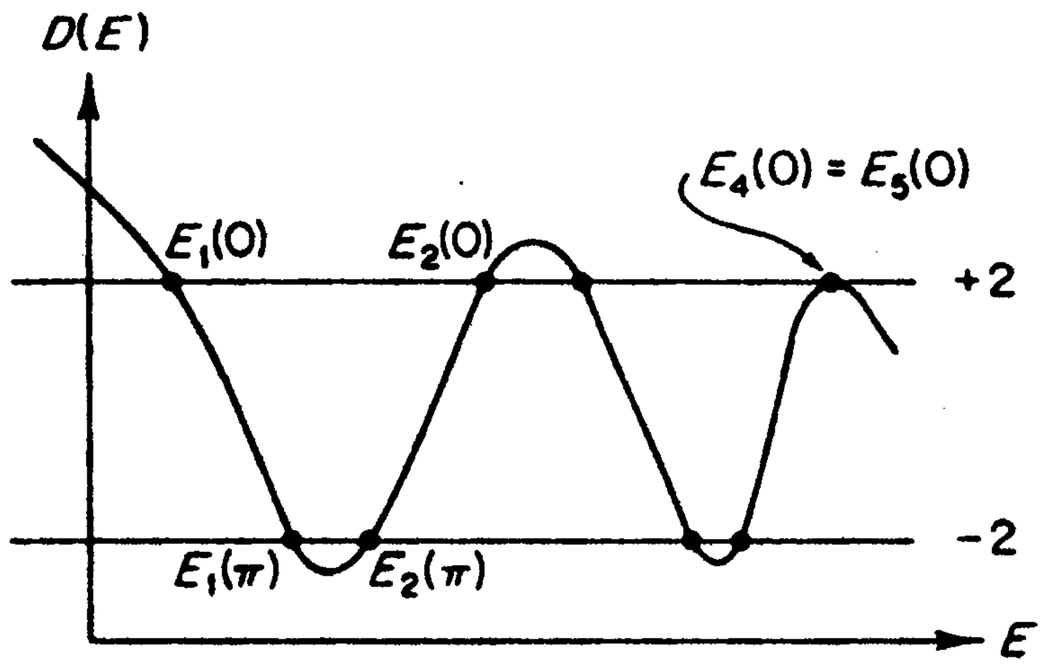


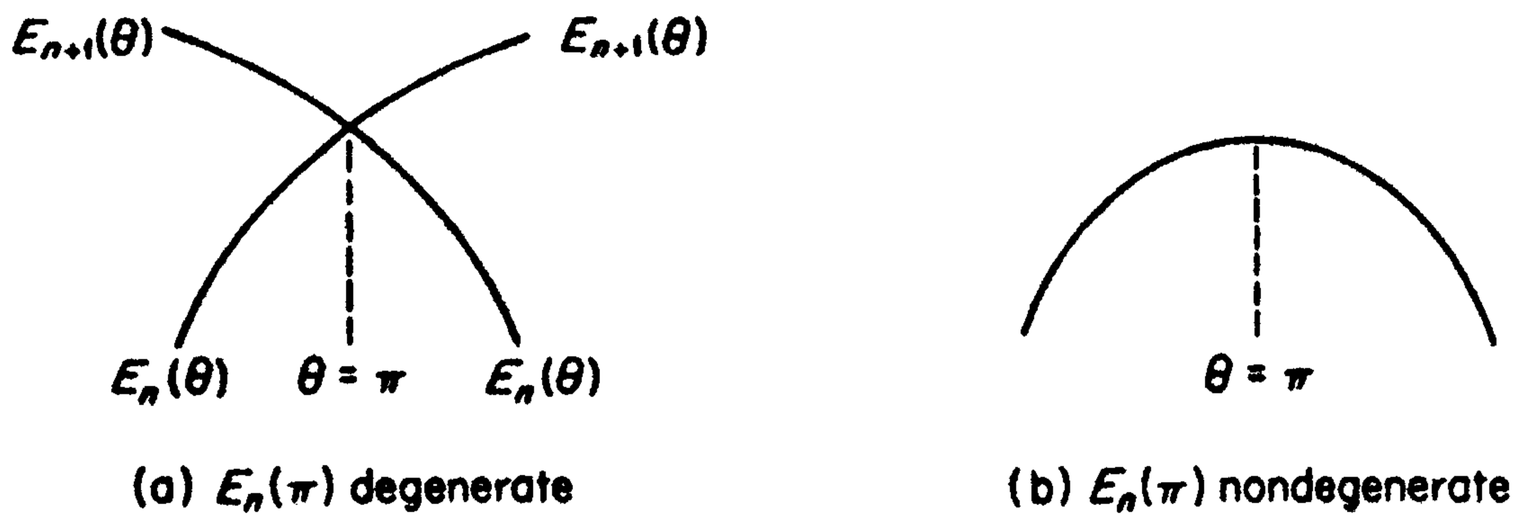
FIGURE XIII.14 A typical discriminant.

We have proven that $E_1(0) \leq E_1(\theta)$ for all θ, so $D(E)$ cannot have any value in $[-2, 2]$ for $E < E_1(0)$. Now $D(E) = 2$ for $E = E_1(0)$. As θ varies from 0 to π, $D(E_1(\theta))$ varies from 2 to -2. E_1 must therefore be strictly monotone increasing since it has an inverse function $\mathrm{Arc}\cos \frac{1}{2}D(E_1(\theta)) = \theta$. We have $D(E_1(\pi)) = -2$. D must eventually turn around (since $H(\pi)$ has additional eigenvalues) so the next value of $D(\theta)$ in $[-2, 2]$ to occur must be -2. This occurs at $E_2(\pi)$ and then D runs from -2 to 2 as θ goes from π to 0. Thus we have the picture in Figure XIII.14. The only subtlety is that we must show that if D has a turning point at $+2$ or -2, then $H(0)$ or $H(\pi)$ has a double eigenvalue. But if $D(E)$ has a turning point at $E = E_0$ with $D(E) = +2$, then for θ near 0, $H(\theta)$ has two eigenvalues near E_0 corresponding to the fact that $D(E) = 2 \cos \theta$ has two solutions near $E = E_0$. By analytic perturbation theory E_0 must be a double eigenvalue of $H(0)$.

(f) This follows from the analytic perturbation theory of Section XII.2. ∎

The reader may have noticed that while we have been careful to avoid saying that $E_n(\theta)$ is analytic near $\theta = \pi$ or 0, it clearly is. However, if $E_n(\theta)$ is

continued through $\theta = \pi$, the continuation may be $E_{n+1}(\theta)$ or $E_{n-1}(\theta)$ if $E_n(\pi)$ is a doubly degenerate eigenvalue (see Figure XIII.15). A similar phenomenon can occur at $\theta = 0$ if we identify θ and $\theta - 2\pi$.



(a) $E_n(\pi)$ degenerate (b) $E_n(\pi)$ nondegenerate

FIGURE XIII.15 Crossed bands.

We can now combine Theorems XIII.85, 86, 88, and 89 to conclude:

Theorem XIII.90 Let V be a piecewise continuous function of period 2π. Let $H = -d^2/dx^2 + V$ on $L^2(\mathbb{R}, dx)$. Let $E_1(0), E_2(0), \ldots$ be the eigenvalues of the corresponding operator on $(0, 2\pi)$ with periodic boundary conditions and let $E_1(\pi), \ldots$ be the eigenvalues with antiperiodic boundary conditions. Let

$$\alpha_n = \begin{cases} E_n(0), & n \text{ odd} \\ E_n(\pi), & n \text{ even} \end{cases} \qquad \beta_n = \begin{cases} E_n(\pi), & n \text{ odd} \\ E_n(0), & n \text{ even} \end{cases}$$

Then:

(a) $\sigma(H) = \bigcup_{n=1}^{\infty} [\alpha_n, \beta_n]$.
(b) H has no eigenvalues.
(c) H has purely absolutely continuous spectrum.

Proof (a) Since the $E_n(\theta)$ are continuous, if θ_0 and ε are given, then for some δ,

$$\{\theta \,|\, |\theta - \theta_0| < \delta\} \subset \{\theta \,|\, |E_n(\theta) - E_n(\theta_0)| < \varepsilon\}$$

so by Theorem XIII.85, $\sigma(H) = \bigcup_n [\alpha_n, \beta_n]$.

(b) No function E_n is constant since the E_n are strictly monotone. Thus for each E_0, $\{\theta \,|\, E_n(\theta) = E_0\}$ is a set with at most two points. Such a set has measure zero, so by Theorem XIII.86, E_0 is not an eigenvalue.

(c) follows by Theorems XIII.86 and 89. ∎

We remark that $-d^2/dx^2 + V$ has a simple eigenfunction expansion, but since we shall give the general n-dimensional result below, we do not pause to give the details now.

The most striking feature of Theorem XIII.90 is that $\sigma(H)$ has gaps $(\beta_1, \alpha_2), \ldots, (\beta_n, \alpha_{n+1}), \ldots$. Of course, all we know is that $\beta_n \leq \alpha_{n+1}$, so that some of the "gaps" listed may be empty. In fact, if $V = 0$, then there are no gaps, so it is necessary to impose some condition on V for any given gap to be nonempty. The beautiful feature of this analysis is that the occurrence of any gap is reduced to a question about the degeneracy of some eigenvalue.

Example 1 (the Mathieu equation) Let

$$V(x) = \mu \cos x$$

with $\mu \neq 0$. We claim that for all n, $\alpha_{n+1} \neq \beta_n$, i.e., every gap occurs. Let H_0^{P} (respectively, H_0^{A}) be $-d^2/dx^2$ on $L^2(0, 2\pi)$ with periodic (respectively, antiperiodic) boundary conditions. We need only show that $H_0^{\mathrm{P}} + V$ and $H_0^{\mathrm{A}} + V$ have no double eigenvalues. We give the proof for $H_0^{\mathrm{P}} + V$; the proof is similar for $H_0^{\mathrm{A}} + V$. Consider the functions $\varphi_n = (2\pi)^{-1/2} e^{inx}$. Then $\varphi_n \in D(H_0^{\mathrm{P}})$ and $H_0^{\mathrm{P}} \varphi_n = n^2 \varphi_n$. If ψ solves $(H_0^{\mathrm{P}} + V)\psi = E\psi$ and $a_n = (\varphi_n, \psi)$, then

$$(n^2 - E)a_n + \tfrac{1}{2}\mu(a_{n+1} + a_{n-1}) = 0 \tag{158a}$$

If η also solves $(H_0^{\mathrm{P}} + V)\eta = E\eta$ and $b_n = (\varphi_n, \eta)$, then

$$(n^2 - E)b_n + \tfrac{1}{2}\mu(b_{n+1} + b_{n-1}) = 0 \tag{158b}$$

Eliminating the $n^2 - E$ term from (158) and using $\mu \neq 0$, we have $b_n a_{n+1} - a_n b_{n+1} = a_n b_{n-1} - b_n a_{n-1}$ so $b_n a_{n+1} - a_n b_{n+1} = c$, where c is some constant. Since $\eta, \psi \in L^2$, $\sum a_n^2 < \infty$, $\sum b_n^2 < \infty$, so $a_n \to 0$ and $b_n \to 0$ as $n \to \infty$. Therefore c must be zero, and thus

$$a_n b_{n+1} = b_n a_{n+1} \tag{159}$$

By (158a), if any two successive a_j are zero, all the a_j are zero so for any n, either $a_n \neq 0$ or $a_{n+1} \neq 0$. A similar result holds for the b_n. Now suppose that E is a doubly degenerate eigenfunction. Since $\cos x$ is even under $x \to -x$, we can choose ψ to be the even solution of $-\psi'' + V\psi = E\psi$ and η to be the odd solution since all solutions are periodic if $H_0^{\mathrm{P}} + V$ has E as a degenerate eigenvalue. Since η is odd, $b_0 = \int_{-\pi}^{\pi} \eta(x)\, dx = 0$. Thus, by our remark above, $b_1 \neq 0$. Since ψ is even, $a_n = a_{-n}$ and so, in particular, by (158a)

$$-Ea_0 + \mu a_1 = 0$$

It follows that $a_0 \neq 0$ since if it were zero, a_1 would be zero, violating the remark above. Thus $a_0 b_1 \neq 0$ but $a_1 b_0 = 0$. This violates (159). We conclude that $H_0^{\mathrm{P}} + V$ has no degenerate eigenvalues.

There is another example in Problem 139 where one can obtain an asymptotic formula for $\ell_n = \alpha_{n+1} - \beta_n$ as $n \to \infty$, which proves that at least for large n (where $\ell_n \neq 0$), there are lots of gaps. There are also the following general results whose proofs can be found in the references in the Notes.

Theorem XIII.91 Let V be periodic of period 2π. Then:

(a) If no gaps are present, V is a constant.
(b) If precisely one gap occurs, then V is a Weierstrass elliptic function.
(c) If all the odd gaps are absent (i.e., if $H_0^{\mathrm{A}} + V$ has only degenerate eigenvalues), then V has period π. More generally, if, for fixed n, all gaps (β_k, α_{k+1}) are absent for $k \neq 2^n m$ $(m = 1, 2, \ldots)$, then V has period $2^{-n}(2\pi)$ and the converse relation is true.
(d) If only finitely many gaps are present, then V is real analytic as a function on $\mathbb{R}$.
(e) Topologize Y, the space of all C^∞ functions on $\mathbb{R}$ with period 2π, with the seminorms $\|f\|_n = \|D^n f\|_\infty$, $n = 0, 1, \ldots$. Then the set of potentials in V for which *all* gaps are nonzero is a dense G_δ set of Y. (See the discussion of "Baire almost every" in the notes to Section III.5.)

There are some general results about when two potentials V and W produce the same energy bands.

Theorem XIII.92 Let V and W be two potentials of period 2π so that $-d^2/dx^2 + V$ and $-d^2/dx^2 + W$, on $[0, 2\pi]$ with periodic boundary conditions, have the same eigenvalues. Then their energy bands are the same.

Proof We shall sketch the main ideas. Fuller details can be found in the reference in the notes. Let $D_V(E)$ and $D_W(E)$ be the respective discriminants. By the analysis used in the proof of Theorem XIII.89, it suffices to prove that the discriminants are equal. We claim that

$$|D_V(E)| + |D_W(E)| \leq C_1 \exp(C_2 |E|^{1/2}) \tag{160}$$

$$D_V(E)/2 \cos(2\pi\sqrt{E}) \to 1 \quad \text{as} \quad E \to i\infty \tag{161}$$

$$D_W(E)/2 \cos(2\pi\sqrt{E}) \to 1 \quad \text{as} \quad E \to i\infty \tag{162}$$

Deferring the proofs of (160)–(162), let us complete the proof that $D_V = D_W$. By (160) and the Hadamard factorization theorem of complex analysis,

$$2 - D_V(E) = C_V \prod_{j=1}^{\infty} (1 - E_j(V)^{-1}E)$$

$$2 - D_W(E) = C_W \prod_{j=1}^{\infty} (1 - E_j(W)^{-1}E)$$

where $E_j(V)$ are the zeros of $D_V(E) - 2$. By hypothesis, the zeros of $2 - D_V$ and $2 - D_W$ are the same. By (161) and (162), $(2 - D_V)/(2 - D_W) \to 1$ as $E \to i\infty$, so $D_V = D_W$.

(160)–(162) follow by a detailed analysis of the solutions $u_j(x, E)$. One shows that they solve integral equations, for example,

$$u_1(x, E) = \cos(x\sqrt{E}) + \frac{1}{\sqrt{E}} \int_0^x \sin((x - y)\sqrt{E})V(y)u_1(y, E)\, dy$$

By iterating these equations, one proves (160)–(162). ∎

At first sight, one might think that there are not many pairs V, W with $D_V = D_W$. Quite the contrary: In the Notes, the reader can find references for the following two theorems:

Theorem XIII.93 Let $V(x, t)$ solve the partial differential equation

$$\frac{\partial V}{\partial t} = 3V\frac{\partial V}{\partial x} - \frac{1}{2}\frac{\partial^3 V}{\partial x^3} \tag{163}$$

with $V(x, 0)$ periodic of period 2π. Then for each fixed t, $V(x, t)$ is periodic of period 2π and has energy bands independent of t.

Equation (163) is called the **Korteweg–de Vries equation.**

Theorem XIII.94 Topologize the C^∞ functions on $\mathbb{R}$ with period 2π by the seminorms $\|D^\alpha f\|_\infty$. Fix V and suppose that the spectrum of $-d^2/dx^2 + V$ has n gaps (n may be infinite). Then $\{W \mid D_V = D_W\}$ is homeomorphic to an n-dimensional torus.

In the one-dimensional case one can also say quite a lot about global analytic properties of $E_n(\theta)$.

Theorem XIII.95 (Kohn's theorem) Suppose that all the gaps in a one-dimensional problem are nonzero. Then the energy band functions $E_n(\theta)$ are the branches of a single multisheeted function that has no singularities other than square root branch points on the lines $\operatorname{Im}\theta = m\pi$, $m = 0, \pm 1, \ldots$. Explicitly, there exist positive numbers $\alpha_1, \alpha_2, \ldots$ so that the Riemann surface of $E(\theta)$ can be described as follows. E is equal to $E_n(\theta)$ on the nth sheet which is cut in $\bigcup_m [(2m+1)\pi] \pm i(\alpha_n, \infty)$ and $\bigcup_m (2m\pi) \pm i(\alpha_{n-1}, \infty)$ for n odd; and $\bigcup_m [2m\pi] \pm i(\alpha_n, \infty)$ and $\bigcup_m [(2m+1)\pi] \pm i(\alpha_{n-1}, \infty)$ for n even. The nth and $(n+1)$th sheet are joined by crossing the cuts $2m\pi \pm i(\alpha_n, \infty)$ (n even) and $(2m+1)\pi \pm i(\alpha_n, \infty)$ (n odd); see Figure XIII.16.

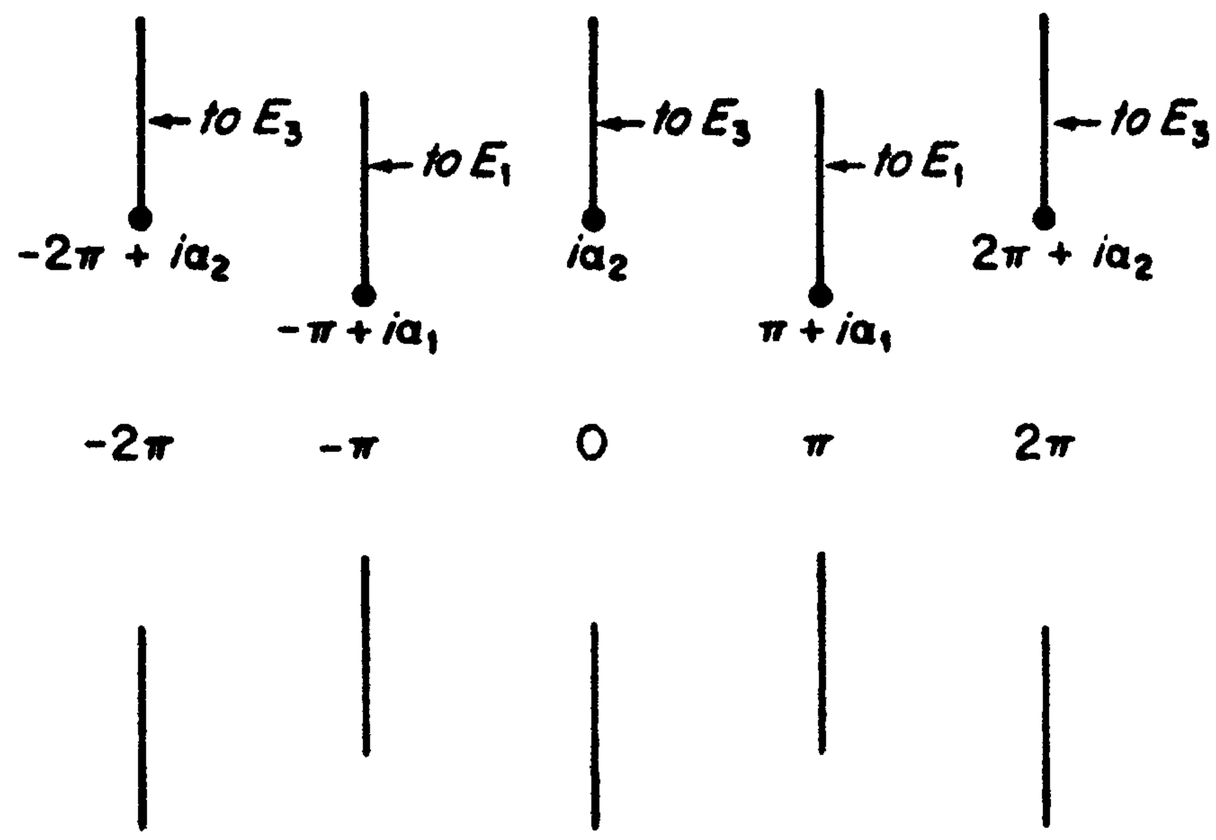


FIGURE XIII.16 The Riemann surfaces of an energy band; $n = 2$.

For a proof of this theorem, see the references in the Notes.

Now we turn to the general n-dimensional case. The direct integral decomposition in both the x-space and p-space versions will go through without significant change. The main difficulty will be in extending the analysis of the fibers of H (Theorem XIII.89). For that analysis depended critically on the simplicity of the eigenvalues of $H(\theta)$, which fails in the multidimensional case. An additional complication is that in the multivariable case, eigenvalues are not necessarily analytic (in a single-valued sense) at degeneracy points: See the example in the Notes to Section XII.1. It will turn out to be easier to analyze the fibers of the direct integral decomposition in the p-space version.

We want to allow for the possibility of local singularities in V in our discussion of the general n-dimensional case. The perturbation criteria, as stated in Section X.2, are not applicable if V is unbounded since such a periodic V cannot be in any $L^p + L^\infty$ with $p < \infty$; but if V is L^p over all bounded sets and periodic, then it will be uniformly locally L^p where:

Definition A measurable function V on $\mathbb{R}^n$ is called **uniformly locally L^p** if and only if

$$\int_C |V(x)|^p \, d^n x \leq A$$

for any unit cube C and some C-independent constant A.

The perturbation theory of Section X.2 extends to uniformly locally L^p perturbations (for suitable p) by the following localization method.

Theorem XIII.96 Let $p = 2$ if $n \leq 3$, $p > 2$ if $n = 4$ and $p > n/2$ if $n \geq 5$. Then any real-valued function on $\mathbb{R}^n$ that is uniformly locally L^p is a $-\Delta$-bounded operator with relative bound zero.

Proof Let q be such that $p^{-1} + q^{-1} = \frac{1}{2}$. We proved in Section X.2 that for any ε, there is an A_ε so that

$$\|\varphi\|_q^2 \leq \varepsilon \|\Delta\varphi\|_2^2 + A_\varepsilon \|\varphi\|_2^2 \tag{164}$$

For any cube C, let

$$\|\varphi\|_{r;C}^r \equiv \int_C |\varphi(x)|^r \, d^n x$$

Let C be a unit cube and let C' be the cube with side 3 and the same center as C. Let η be a C^∞ function with support in C' that is identically 1 on C. Now, by (164),

$$\begin{aligned} \|\varphi\|_{q,C}^2 &\leq \|\eta\varphi\|_q^2 \\ &\leq \varepsilon \|\Delta(\eta\varphi)\|_2^2 + A_\varepsilon \|\eta\varphi\|_2^2 \\ &\leq 3\varepsilon \|\Delta\varphi\|_{2;C'}^2 + B\|\nabla\varphi\|_{2;C'}^2 + D\|\varphi\|_{2;C'}^2 \end{aligned} \tag{165}$$

where we have used $\Delta(\eta\varphi) = \varphi\,\Delta\eta + \eta\,\Delta\varphi + 2\,\nabla\eta \cdot \nabla\varphi$, the triangle inequality, the fact that $(a+b+c)^2 \leq 3(a^2+b^2+c^2)$, and the fact that η, $\nabla\eta$, and $\Delta\eta$ are bounded functions with support in C'. Notice that since the various $\|D^\alpha\eta\|_\infty$ can be chosen independently of C, (165) holds with constants that are independent of C. For $\alpha \in \mathbb{Z}^n$, let C_α be the unit cube with center α and C'_α the corresponding C'. Then, since V is uniformly locally L^p,

$$|||V|||^2 \equiv \sup_\alpha \|V\|_{p,C_\alpha}^2 < \infty$$

Thus,

$$\begin{aligned}\|V\varphi\|_2^2 &= \sum_\alpha \|V\varphi\|_{2;C_\alpha}^2 \\ &\le \sum_\alpha \|V\|_{p;C_\alpha}^2 \|\varphi\|_{q;C_\alpha}^2 \\ &\le |||V|||^2 \sum_\alpha (3\varepsilon\|\Delta\varphi\|_{2;C_{\alpha'}}^2 + B\|\nabla\varphi\|_{2;C_{\alpha'}}^2 + D\|\varphi\|_{2;C_{\alpha'}}^2) \\ &= |||V|||^2 3^n (3\varepsilon\|\Delta\varphi\|_2^2 + B\|\nabla\varphi\|_2^2 + D\|\varphi\|_2^2) \\ &\le |||V|||^2 3^n (4\varepsilon\|\Delta\varphi\|_2^2 + (D + \tfrac{1}{4}\varepsilon^{-1}B)\|\varphi\|_2^2)\end{aligned}$$

In the next to the last step, we have used the fact that each $x \in \mathbb{R}^n$ not on the boundary of some C_α lies in precisely 3^n of the C'_α. Then, in the last step we used,

$$\|\nabla\varphi\|_2^2 \le \delta\|\Delta\varphi\|_2^2 + \tfrac{1}{4}\delta^{-1}\|\varphi\|_2^2$$

which via the Plancherel theorem follows by the numerical inequality $a \le \delta a^2 + \frac{1}{4}\delta^{-1}$. ∎

Notice that if V is uniformly locally L^p for some $p > n/2$ then it is automatically uniformly locally $L^{n/2}$ so we stated $p = n/2$ rather than $p \ge n/2$ in the above theorem.

Given the above criterion, the following theorem has a proof that differs only in notation from the corresponding one-dimensional result (Theorem XIII.88).

Theorem XIII.97 Let $\mathbf{a}_1, \ldots, \mathbf{a}_n$ be n independent vectors in $\mathbb{R}^n$. Let V be a real-valued function on $\mathbb{R}^n$ obeying:

(i) $V(\mathbf{x} + \mathbf{a}_i) = V(\mathbf{x})$, $i = 1, \ldots, n$.

(ii) $\int_Q |V(\mathbf{x})|^p \, d^n x < \infty$ where Q is a **basic period cell**

$$Q = \left\{ \mathbf{x} \,\middle|\, \mathbf{x} = \sum_{i=1}^n t_i \mathbf{a}_i; 0 \le t_i < 1 \right\}$$

and $p = 2$ if $n \le 3$, $p > 2$ if $n = 4$; $p = n/2$ if $n \ge 5$.

For each $\boldsymbol{\theta} \in [0, 2\pi)^n$, let $H^{(0)}(\boldsymbol{\theta})$ be the operator $-\Delta$ on $L^2(Q, d^n x) \equiv \mathscr{H}$ with the boundary conditions

$$\varphi(\mathbf{x} + \mathbf{a}_j) = e^{i\theta_j}\varphi(\mathbf{x}), \qquad \frac{\partial\varphi}{\partial y_j}(\mathbf{x} + \mathbf{a}_j) = e^{i\theta_j}\frac{\partial\varphi}{\partial y_j}(\mathbf{x}) \tag{166}$$

for all $\mathbf{x}$ with $\mathbf{x}, \mathbf{x} + \mathbf{a}_j \in \bar{Q}$ (i.e., for $\mathbf{x}$ on suitable faces of ∂Q where y_j is the coordinate given by $\mathbf{x} = \sum y_i \mathbf{a}_i$. Let

$$\mathscr{H} = \int_{[0, 2\pi)^n}^{\oplus} \mathscr{H}' \frac{d^n\theta}{(2\pi)^n}$$

and let $U: L^2(\mathbb{R}^n, d^nx) \to \mathscr{H}$ by defining U on $\mathscr{S}$ by

$$(Uf)_{\boldsymbol{\theta}}(\mathbf{x}) = \sum_{m \in \mathbb{Z}^n} e^{-i\boldsymbol{\theta} \cdot \mathbf{m}} f(\mathbf{x} + \sum m_i \mathbf{a}_i)$$

and extended as a unitary operator to L^2.

Then:

(a) For almost all $\boldsymbol{\theta} \in [0, 2\pi)^n$, V is an $H^{(0)}(\boldsymbol{\theta})$-bounded multiplication operator on $L^2(Q, d^nx)$ with relative bound zero.

(b) $U(-\Delta + V)U^{-1} = \int_{[0, 2\pi)^n}^{\oplus} H(\boldsymbol{\theta})\, d^n\theta/(2\pi)^n$ where $H(\boldsymbol{\theta}) = H^{(0)}(\boldsymbol{\theta}) + V$.

We remark that it is possible to prove that V is everywhere, and not just almost everywhere, $H^{(0)}(\boldsymbol{\theta})$-bounded with relative bound zero. This follows, for example, from analyticity arguments.

One consequence of this theorem is the existence of an eigenfunction expansion for H in the sense of Section XI.6:

Theorem XIII.98 Each $H(\boldsymbol{\theta})$ has a complete set of eigenfunctions $\psi_m(\boldsymbol{\theta}; x)$ with eigenvalues $E_m(\boldsymbol{\theta})$. Extend $\psi_m(\boldsymbol{\theta}; x)$ to all of $\mathbb{R}^n$ by using the boundary condition (166). For $\varphi \in \mathscr{S}(\mathbb{R}^n)$, let

$$\tilde{\varphi}(m; \boldsymbol{\theta}) = \int_{\mathbb{R}^n} \overline{\psi_m(\boldsymbol{\theta}; x)}\, \varphi(x)\, d^nx$$

Then:

(a) $$\int_{\mathbb{R}^n} |\varphi(x)|^2\, d^nx = \sum_m \int_{[0, 2\pi)^n} |\tilde{\varphi}(m; \boldsymbol{\theta})|^2 \frac{d^n\theta}{(2\pi)^n}$$

(b) $$\varphi(x) = \frac{1}{(2\pi)^n} \sum_m \int_{[0, 2\pi)^n} \tilde{\varphi}(m; \boldsymbol{\theta}) \psi_m(\boldsymbol{\theta}; x)\, d^n\theta$$

(c) Extend $\tilde{}$ to $L^2(\mathbb{R}^n)$ by continuity. Then $H = -\Delta + V$ obeys

$$\widetilde{H\varphi}(m; \boldsymbol{\theta}) = E_m(\boldsymbol{\theta}) \tilde{\varphi}(m; \boldsymbol{\theta})$$

for all $\varphi \in D(H)$.

(d) $\tilde{}$ maps $L^2(\mathbb{R}^n, d^nx)$ *onto* $\bigoplus_m L^2([0, 2\pi)^n, d^n\theta)$.

Proof It is possible to find a complete set of eigenvectors for $H^{(0)}(\boldsymbol{\theta})$ explicitly; namely,

$$\psi_{\mathbf{k}}^{(0)}(\boldsymbol{\theta}; x) = (2\pi)^{-n/2} \exp\left[i \sum_{j=1}^{n} (\theta_j + 2\pi k_j) y_j\right]$$

for $k_j \in \mathbb{Z}^n$, where y_j is defined by $\mathbf{x} = \sum_{i=1}^{n} y_i \mathbf{a}_i$. The corresponding eigenvalues tend toward infinity as $|\mathbf{k}| \to \infty$ so $H^{(0)}(\boldsymbol{\theta})$ has compact resolvent. It follows that $H(\boldsymbol{\theta})$ has compact resolvent by Theorem XIII.68. Thus it has discrete eigenvalues $\{E_m(\boldsymbol{\theta})\}_{m=1}^{\infty}$ and a corresponding complete set of eigenfunctions. By the min–max principle, one can prove that the functions $E_m(\boldsymbol{\theta})$ are measurable and that the corresponding eigenfunctions can be chosen measurably (Problem 140). Since, for $\boldsymbol{\theta}$ fixed, the $\psi_m(\boldsymbol{\theta})$ are an orthonormal basis in $\mathscr{H}'$ of eigenfunctions for $H(\boldsymbol{\theta})$, we have for $\eta \in \mathscr{H} = \int_{[0, 2\pi)^n}^{\oplus} \mathscr{H}' \, d^n\theta/(2\pi)^n$,

$$(\eta, \eta)_{\mathscr{H}} = \sum_m \int |(\eta_{\boldsymbol{\theta}}, \psi_m(\boldsymbol{\theta}))_{\mathscr{H}'}|^2 \frac{d^n\theta}{(2\pi)^n}$$

$$\eta_{\boldsymbol{\theta}} = \sum_m (\psi_m(\boldsymbol{\theta}), \eta_{\boldsymbol{\theta}})_{\mathscr{H}'} \psi_m(\boldsymbol{\theta})$$

$$(\psi_m(\boldsymbol{\theta}), (A\eta)_{\boldsymbol{\theta}}) = E_m(\boldsymbol{\theta})(\psi_m(\boldsymbol{\theta}), \eta_{\boldsymbol{\theta}})$$

where

$$A = \int_{[0, 2\pi)^n}^{\oplus} H(\boldsymbol{\theta}) \frac{d^n\theta}{(2\pi)^n}$$

(a)–(c) now follow using the definition of U and the way we have extended $\psi_m(\boldsymbol{\theta})$. (d) has a similar proof. ∎

To give the p-space analysis, we need a definition that differs by a factor of 2π from the more common one.

Definition Let $\mathbf{a}_1, \ldots, \mathbf{a}_n$ be a basis for $\mathbb{R}^n$. The **dual basis** $\mathbf{K}_1, \ldots, \mathbf{K}_n$ is defined by

$$(\mathbf{K}_i, \mathbf{a}_j) = (2\pi)\delta_{ij}$$

Theorem XIII.99 Let V be a function on $\mathbb{R}^n$ with $V(\mathbf{x} + \mathbf{a}_j) = V(\mathbf{x})$ $(j = 1, \ldots, n)$ where $\{\mathbf{a}_j\}_{j=1}^{n}$ is a basis for $\mathbb{R}^n$. Let Q be the basic period cell for the basis $\{\mathbf{a}_i\}$ and let $\tilde{Q}$ be the basic period cell for the dual basis $\{\mathbf{K}_i\}$, i.e.,

$$\tilde{Q} = \left\{ \sum_{i=1}^{n} t_i \mathbf{K}_i \,\middle|\, 0 \le t_i < 1 \right\}$$

Let $\mathscr{H}' = \ell_2(\mathbb{Z}^n)$ and $\mathscr{H} = \int_Q^\oplus \mathscr{H}'\, d^n k$. Suppose that V is uniformly locally L^p (with $p = 2$ if $n \le 3$, $p > 2$ if $n = 4$, $p = n/2$ if $n \ge 5$) and let $\tilde{V}_{\mathbf{m}}$ be the Fourier coefficients for V as a function on Q; i.e., for $\mathbf{m} \in \mathbb{Z}^n$,

$$\tilde{V}_{\mathbf{m}} = (\text{vol}\, Q)^{-1} \int_Q \exp\left(-i \sum_{j=1}^n m_j \mathbf{K}_j \cdot \mathbf{x}\right) V(\mathbf{x})\, d^n x \tag{167}$$

For $\mathbf{k} \in \tilde{Q}$, define the operator $H(\mathbf{k})$ on $\mathscr{H}'$ by

$$(H(\mathbf{k})g)_{\mathbf{m}} = (\mathbf{k} + \sum m_j \mathbf{K}_j)^2 g_{\mathbf{m}} + \sum_{\alpha \in \mathbb{Z}^n} \tilde{V}_\alpha g_{\mathbf{m}-\alpha} \tag{168}$$

with domain

$$D_0 = \{g \in \mathscr{H}' \,|\, \sum \mathbf{m}^2 |g_{\mathbf{m}}|^2 < \infty\}$$

Finally, let $U: L^2(\mathbb{R}^n) \to \mathscr{H}$ by

$$[(Uf)(\mathbf{k})]_{\mathbf{m}} = \hat{f}(\mathbf{k} + \sum m_j \mathbf{K}_j)$$

Then U is unitary and

$$U(-\Delta + V)U^{-1} = \int_{\tilde{Q}}^\oplus H(\mathbf{k})\, d^n k$$

Proof That U is unitary is just the Plancherel theorem. Moreover, it is clear that

$$[(U(-\Delta)U^{-1})g](\mathbf{k})_{\mathbf{m}} = (\mathbf{k} + \sum m_j \mathbf{K}_j)^2 g(\mathbf{k})_{\mathbf{m}}$$

since $-\widehat{\Delta f}(\ell) = \ell^2 \hat{f}(\ell)$. Because V is $-\Delta$-bounded with relative bound zero, we need only prove that

$$[(UVU^{-1}g)(\mathbf{k})]_{\mathbf{m}} = \sum_{\alpha \in \mathbb{Z}^n} V_\alpha g_{\mathbf{m}-\alpha}(\mathbf{k})$$

and this follows if we prove that, for $f \in \mathscr{S}(\mathbb{R}^n)$,

$$\widehat{Vf}(k) = \sum_{\alpha \in \mathbb{Z}^n} \tilde{V}_\alpha \hat{f}\left(\mathbf{k} - \sum_{j=1}^n \alpha_j \mathbf{K}_j\right) \tag{169}$$

To prove (169) we need only show that, as a tempered distribution, V has the Fourier transform

$$\hat{V}(\mathbf{k}) = (2\pi)^{n/2} \sum_{\alpha \in \mathbb{Z}^n} \tilde{V}_\alpha\, \delta\left(\mathbf{k} - \sum_{j=1}^n \alpha_j \mathbf{K}_j\right)$$

As in the one-dimensional case, this is true because the Fourier series

$$V(\mathbf{x}) = \sum_{\alpha \in \mathbb{Z}^n} \tilde{V}_\alpha\, \exp\left(i \sum_{j=1}^n \alpha_j \mathbf{K}_j \cdot \mathbf{x}\right)$$

is locally L^2 convergent since V is locally uniformly L^2. ∎

One advantage of the k-space decomposition in the form we have presented it is that the operators $H(\mathbf{k})$ have a fixed domain D_0. In fact, we can use (168) to define $H(\mathbf{k})$ for any $\mathbf{k} \in \mathbb{C}^n$ and $H(\mathbf{k})$ so defined is an entire analytic family of type (A). The easiest way of seeing this is to let

$$(\mathbf{P}g)_{\mathbf{m}} = \left(\sum_{j=1}^{n} m_j \mathbf{K}_j\right) g_{\mathbf{m}}$$

so that $\mathbf{P}$ is $H(\mathbf{0})$-bounded with relative bound zero and

$$H(\mathbf{k}) = H(\mathbf{0}) + 2\mathbf{k} \cdot \mathbf{P} + \sum_{j=1}^{n} k_j^2 \tag{170}$$

$H(\mathbf{k})$ depends on n parameters; but it is useful to fix $n-1$ of them for two reasons. First, we avoid the nonanalyticity that can occur in real multiparameter eigenvalue variations. The second reason is more subtle. Let $\mathbf{a}$ and $\mathbf{b}$ be fixed vectors in $\mathbb{R}^n$. Let $z = \lambda + iy$ and define

$$E_{\mathbf{m}}(z) = (\mathbf{a} + z\mathbf{b} + \sum m_j \mathbf{K}_j)^2$$

Of course $H(\mathbf{k}) = H_0(\mathbf{k}) + V$ where $H_0(\mathbf{a} + z\mathbf{b})$ has a complete orthogonal set of eigenvectors with eigenvalues $E_{\mathbf{m}}(z)$. Now

$$\text{Im } E_{\mathbf{m}}(z) = 2y[\mathbf{b} \cdot (\mathbf{a} + \lambda\mathbf{b} + \sum m_j \mathbf{K}_j)]$$

is especially simple if the numbers $\mathbf{b} \cdot \mathbf{K}_j$ are rationally dependent for in that case the number in square brackets will not get arbitrarily small as $\mathbf{m}$ varies. It is thus convenient to pick $\mathbf{b}$ as the first vector in the x-space lattice, i.e.,

$$\mathbf{b} \cdot \mathbf{K}_j = 2\pi\delta_{j1} \tag{171}$$

and λ by

$$\mathbf{b} \cdot (\mathbf{a} + \lambda\mathbf{b}) = \pi \tag{172}$$

In that case, $\text{Im } E_{\mathbf{m}}(z) = 2\pi y(2m_1 + 1)$, so

$$|\text{Im } E_{\mathbf{m}}(z)| \geq \pi|y|(1 + |m_1|) \tag{173a}$$

Moreover, it is easy to see that (Problem 141a)

$$|\text{Re}(E_{\mathbf{m}}(z) + 1)| \geq c_1|\mathbf{m}|^2 \quad \text{if} \quad |\mathbf{m}| \geq c_2(1 + |y|) \tag{173b}$$

for suitable c_1 and c_2 (which will depend on $\mathbf{a}$ through the choice of λ in (172)). From (173), one deduces that (Problem 141):

Lemma 1 Let $n \geq 2$. Let $\mathbf{b}$ be given by (171) and λ by (172). Then

(a) If $\alpha > \frac{1}{2}n$ and $\alpha \geq n - 1$,

$$f_\alpha(y) \equiv \sum_{\mathbf{m}} |E_{\mathbf{m}}(\lambda + iy) + 1|^{-\alpha}$$

is convergent and bounded for $|y| \geq 1$.

(b) If moreover $\alpha > n - 1$, then $\lim_{y \to \pm\infty} f_\alpha(y) = 0$.

The point of Lemma 1 is that it will allow us to control $\|V(H_0(\lambda + iy) + 1)^{-1}\|$ as $y \to \infty$ for suitable V's.

Lemma 2 Let $n \geq 2$. Let V be a periodic potential whose Fourier coefficients (167) obey

$$\sum_{\mathbf{m}} |\tilde{V}_{\mathbf{m}}|^\beta < \infty \tag{174}$$

where $\beta < (n-1)/(n-2)$ if $n \geq 3$ and $\beta = 2$ if $n = 2$. Fix $\mathbf{a} \in \mathbb{R}^n$ and let $\mathbf{b}$ obey (171). Let

$$A(t) = H(\mathbf{a} + \mathbf{b}t)$$

for $t \in \mathbb{R}$. Then:

(a) Each $A(t)$ has compact resolvent.

(b) There are real analytic functions $\{E_j(t)\}$ and corresponding analytic vector-valued functions $\psi_j(t)$ so that $\psi_j(t)$ is a basis for $\mathscr{H}' = \ell^2(\mathbb{Z}^n)$ and, for each t,

$$A(t)\psi(t) = E_j(t)\psi_j(t)$$

(c) No $E_j(t)$ is constant.

Proof (a) Since $\beta \leq 2$, (174) and the Hausdorff–Young inequality imply that V is in $L^\alpha(Q)$ where $\alpha < n - 1$ if $n \geq 3$ and $\alpha = 2$ if $n = 2$. Thus V is $H_0(\mathbf{k})$ relatively bounded so it suffices to prove that $H_0(\mathbf{k})$ has compact resolvent. This follows from the fact that $H_0(\mathbf{k})$ has a complete set of eigenvectors with eigenvalues going to infinity.

(b) Let $E_j(0)$ be the eigenvalues of $A(t = 0)$, ordered so that $E_1(0) \leq E_2(0) \leq \cdots$. Now, we can continue the eigenvalues and eigenvectors using, if necessary, degenerate perturbation theory. As in the one-dimensional case, we need only show that $E_j(t)$ does not go to infinity at some finite t to conclude that a continuation is possible for all t. By (170)

$$\frac{dA(t)}{dt} = 2(\mathbf{b} \cdot \mathbf{P} + \mathbf{b} \cdot (\mathbf{a} + t\mathbf{b}))$$

so, by first-order perturbation theory, and the fact that $\mathbf{P}$ is $H_0(\mathbf{k})$-bounded,

$$\left| \frac{dE_j(t)}{dt} \right| \leq c(|E_j(t)| + |t| + 1)$$

from which it follows that $E_j(t)$ cannot blow up at finite *real* t.

(c) By Lemma 1, the hypothesis on V, Hölder's inequality and Young's inequality,

$$\lim_{y \to \infty} \|(A_0(\lambda + iy) + 1)^{-1}\| = 0$$

$$\lim_{y \to \infty} \|V[A_0(\lambda + iy) + 1]^{-1}\| = 0$$

where λ is chosen so that (172) holds. From these results and standard perturbation arguments we see that for $|y| \geq Y_0$, $(A(\lambda + iy) + 1)^{-1}$ exists and

$$\lim_{y \to \infty} \|[A(\lambda + iy) + 1]^{-1}\| = 0 \tag{175}$$

Now suppose that some $E_j(t)$ is a constant C for all t. Since $A(t)$ has compact resolvent for all real t, it has a compact resolvent for all $t \in \mathbb{C}$ so that C is always an eigenvalue of $A(t)$. It follows that $(C + 1)^{-1}$ is always an eigenvalue of $(A(t) + 1)^{-1}$ so that

$$\|(A(t) + 1)^{-1}\| \geq (C + 1)^{-1}$$

This violates (175), so no $E_j(t)$ can be constant. ∎

We are now able to give a complete analysis of the spectral properties of Schrödinger operators with periodic potentials:

Theorem XIII.100 Let V be a periodic potential whose Fourier *series* coefficients are in ℓ_β where $\beta < (n-1)/(n-2)$ if $n \geq 3$, $\beta = 2$ if $n = 2, 3$. Then $-\Delta + V$ has purely absolutely continuous spectrum.

Proof $\mathbf{b}, \mathbf{K}_2, \ldots, \mathbf{K}_n$ form a basis for $\mathbb{R}^n$, so we can write the interior of $\tilde{Q}$ in terms of a decomposition $\mathbf{k} = s_1 \mathbf{b} + \cdots + s_n \mathbf{K}_n$ as $\{\langle s_1, s_\perp \rangle | s_1 \in M(s_\perp), s_\perp \in N\}$ where for every $s_\perp \in N$, $M(s_\perp)$ is an open connected set (Figure XIII.17). We can write

$$H = \int_{s_\perp \in N} \int_{s_1 \in M(s_\perp)} H(s_1 \mathbf{b} + \cdots + s_n \mathbf{K}_n)\, ds_1\, d^{n-1}s$$

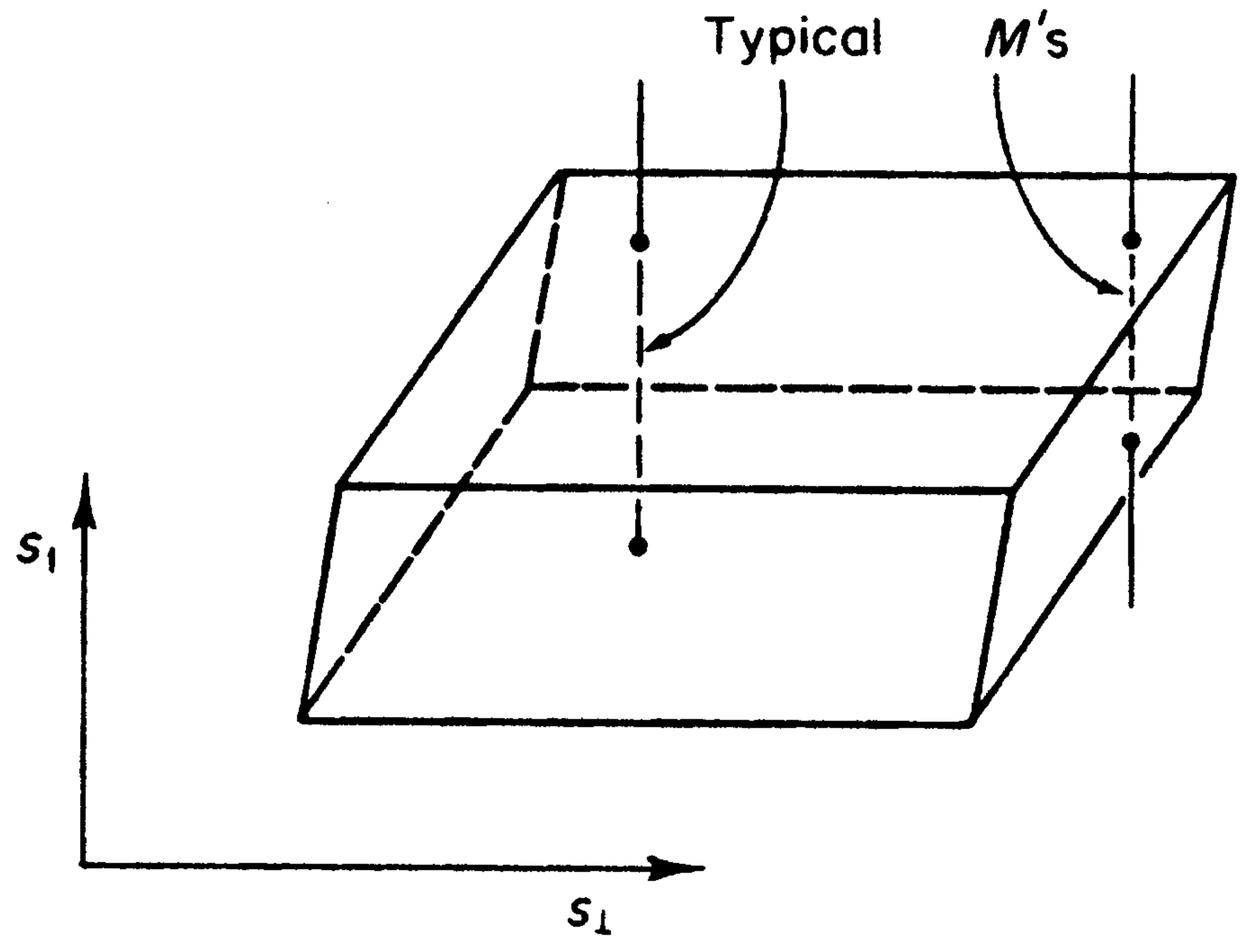


FIGURE XIII.17 The s decomposition of $\tilde{Q}$.

in a suitable direct integral decomposition. By Lemma 2 and Theorem XIII.86, the s_1 direct integral has purely absolutely continuous spectrum for each $s_\perp \in N$ and thus, by Theorem XIII.85f, H has purely absolutely continuous spectrum. ∎

We note that as in the one-dimensional case, the spectrum of H breaks up into "bands," but there are two big differences. First, due to degeneracy there may be some ambiguity in definition at singularities in the many-variable functions. Secondly, bands can "overlap" unlike the one-dimensional case.

Before discussing some of the connections between the ideas above and a simple model of solid state physics, we want to mention an arbitrariness in choice of $\mathbf{a}_1, \ldots, \mathbf{a}_n$. Given V, what is determined without any choice is

$$\mathscr{L}_V = \{\mathbf{a} \,|\, V(\mathbf{x} + \mathbf{a}) = V(\mathbf{x}), \text{ a.e. in } \mathbf{x}\}$$

For periodic potentials, $\mathscr{L}_V$ is always a lattice where:

Definition A **lattice** is a subset $\mathscr{L}$ of $\mathbb{R}^n$ obeying:

(i) $\mathscr{L}$ is discrete, i.e., it has no finite limit points.
(ii) $\mathscr{L}$ is a subgroup of the additive group of $\mathbb{R}^n$.
(iii) No proper vector subspace of $\mathbb{R}^n$ contains $\mathscr{L}$.

Any such $\mathscr{L}$ has a **basis**, i.e., a set $\mathbf{a}_1, \ldots, \mathbf{a}_n \in \mathscr{L}$, so that any $\mathbf{a} \in \mathscr{L}$ is uniquely of the form $\mathbf{a} = \sum_{i=1}^n m_i \mathbf{a}_i$ with $m_i \in \mathbb{Z}$. Such bases are not unique and the corresponding basic period cell Q is not unique; for example, see Figure XIII.18. What all basic cells have in common is the property that $\mathbb{R}^n = \bigcup_{\mathbf{a} \in \mathscr{L}} \overline{\tau_\mathbf{a} Q}$, where $\tau_\mathbf{a} S = \{\mathbf{x} + \mathbf{a} \,|\, \mathbf{x} \in S\}$, with $\tau_\mathbf{a} Q^{\text{int}} \cap \tau_\mathbf{b} Q^{\text{int}} = \varnothing$, if

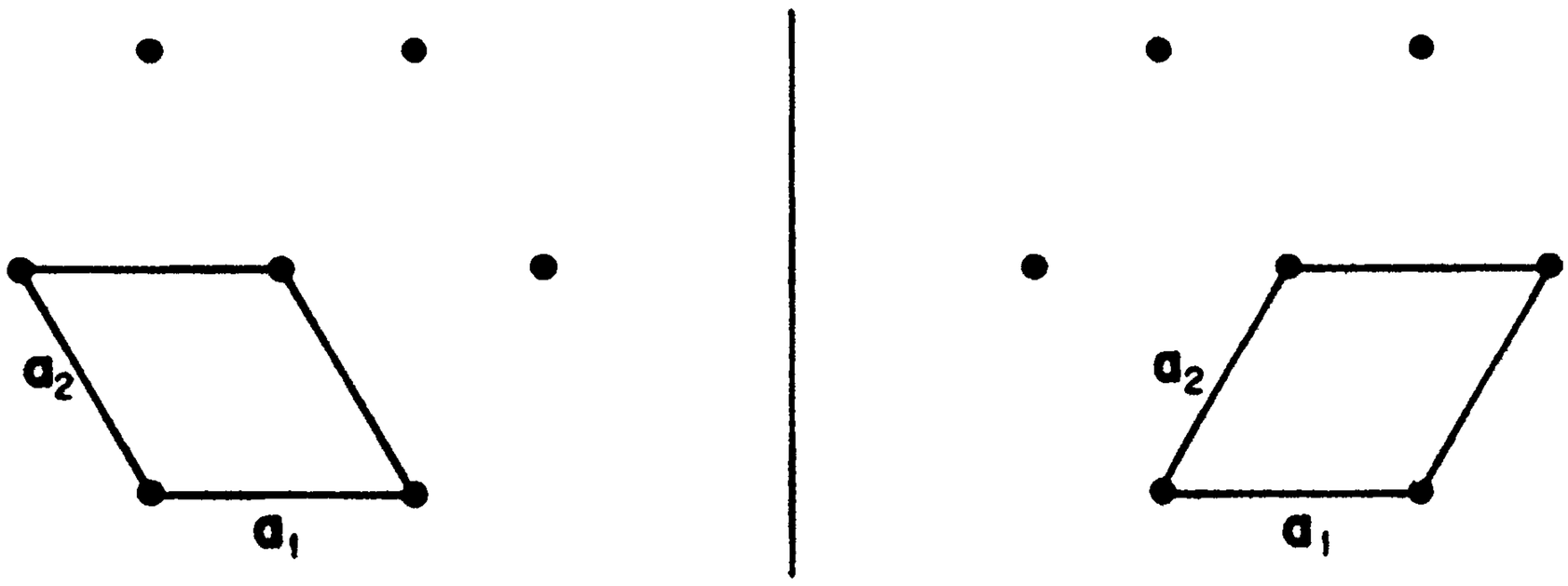


FIGURE XIII.18 Two choices of basis and basic cell.

$\mathbf{a} \neq \mathbf{b}$. There is another "basic cell," C with this property, although it is not associated to any basis. This is the **Wigner–Seitz cell for** $\mathscr{L}$ defined by

$$C = \{x \in \mathbb{R}^n \,|\, x \text{ is closer to 0 than any other point of } \mathscr{L}\}$$

Two examples of Wigner–Seitz cells are shown in Figure XIII.19. One can

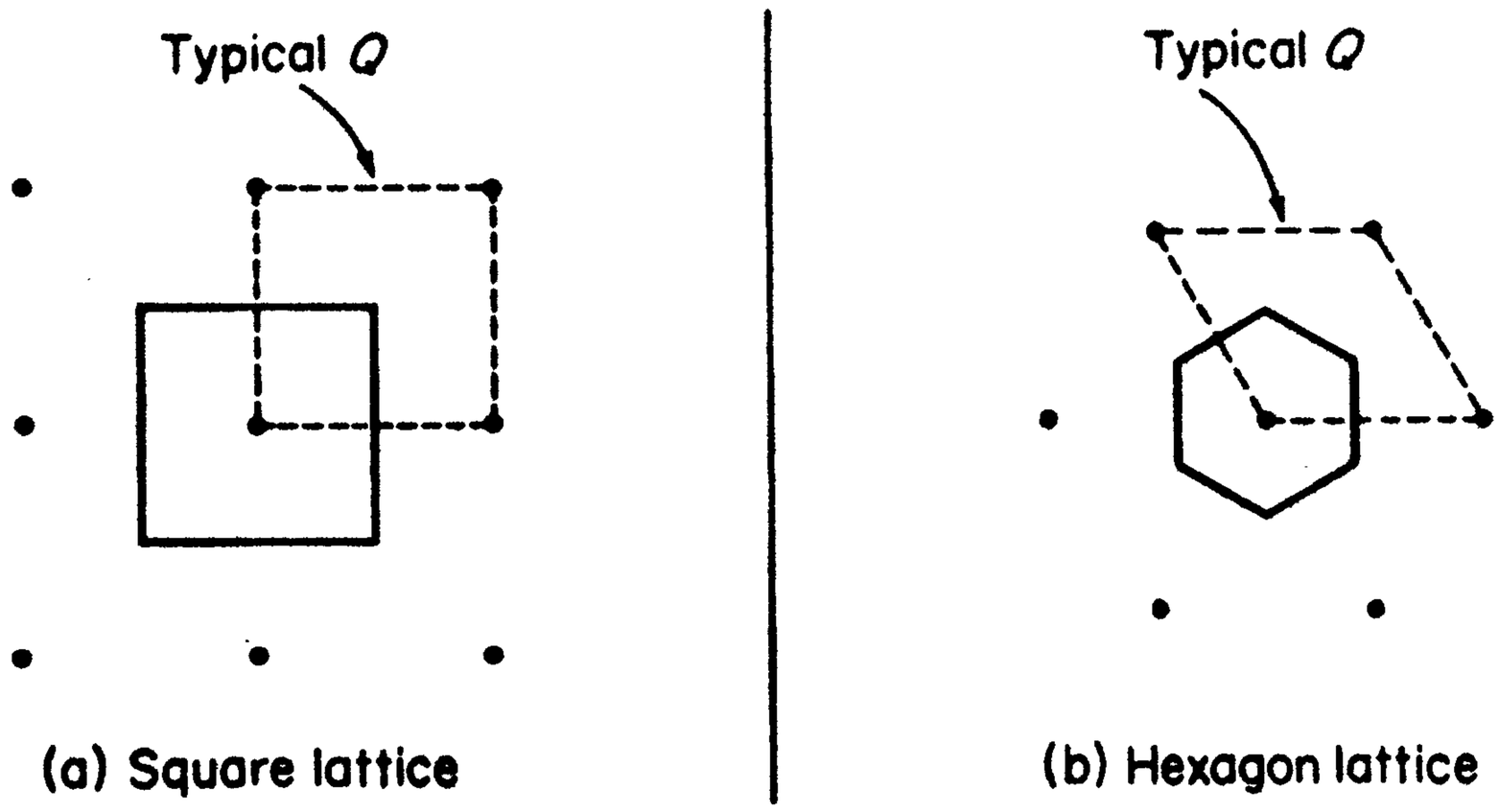


FIGURE XIII.19 Two Wigner–Seitz cells.

show (Problem 143) that any Wigner–Seitz cell is a polyhedron, i.e., the intersection of finitely many slabs $\{x \,|\, a \leq \ell(x) \leq b\}$, ℓ a linear functional. The Wigner–Seitz cell is unique.

Similarly, the dual basis depends on the choice of basis for $\mathscr{L}_V$; but the dual lattice $\mathscr{L}'_V = \{\mathbf{k} \in \mathbb{R}^n \,|\, \mathbf{k} \cdot \mathbf{a} \in 2\pi\mathbb{Z} \text{ for all } \mathbf{a} \in \mathscr{L}\}$ and its Wigner–Seitz cell, called the **Brillouin zone** B, are independent of the basis chosen.

We mention the above terminology for the following reason. One can make an x-space direct integral decomposition with Q replaced by C and a p-space decomposition with $\tilde{Q}$ replaced by B. The study of solids in the physics literature usually begins with a construction that is a disguised form of the p-space direct integral decomposition over the Brillouin zone.

We now turn to applications of our analysis to solid state physics. To the mathematical physicist who is used to looking at atomic physics or even quantum field theory, the bewildering array of approximations known as

solid state theory often appears to be more an art than a science. While there is some truth in this attitude, we would like to emphasize that the difference between atomic physics and solid state physics is really one of degree, for the "standard" purely Coulomb atomic Hamiltonian is an approximation to "real" atoms. In the first place, relativistic corrections to the kinetic energy are not included nor is spin–orbit coupling. In addition, experiments on atoms are not done with isolated atoms but with aggregates, so it is an approximation to discuss a simple atomic model and then compare it with experiment. Finally, there are the couplings to the radiation field (quantum electrodynamics) which are certainly not understood at a fundamental level. The big difference between atomic and solid state physics is that in atomic physics one model describes the most basic physical phenomena, while in solid state physics the model as described below explains qualitatively only a limited range of phenomena. Many phenomena require one to take into account lattice vibrations ("phonons") and interactions between electrons and of the electrons with the phonons. In the end, the mathematical physicist is presented with a well-defined model (or several well-defined models) to study and this is all that he or she can reasonably demand.

It is an observed phenomenon that the nuclei in a solid lie more or less in regular arrays (crystals), i.e., there is a lattice in $\mathbb{R}^n$ so that the nuclei more or less lie at the lattice points. No one has given an explanation from first principles of why crystals form; i.e., no one has proven that a large number of heavy nuclei with enough electrons to produce neutrality, interacting via Coulomb potentials, have a ground state that is approximately a crystal. We thus postulate in our model that there is a *fixed* nucleus with a number of core electrons at each site of a lattice. To obtain simplicity we replace a large solid by one filling all of $\mathbb{R}^n$. Thus if we ignore electron–electron interactions, we have electrons moving under a Hamiltonian $-\Delta + V$ with V periodic. This model is known as the **one-electron model of solids**. We want to use our analysis of periodic Schrödinger operators to describe two things:

(1) the notion of density of states and the qualitative explanation of the difference between metals and insulators;
(2) impurity scattering in the one electron model.

For simplicity of notation we suppose that space is three dimensional.

Definition Let $\tilde{Q}$ be a basic period cell in the dual lattice and let $E_n(\mathbf{k})$ be the energy levels of $H(\mathbf{k})$ (ordered by $E_1 \leq E_2 \leq \cdots$). The **density of states measure** ρ is the measure on $\mathbb{R}$ defined by

$$\rho(-\infty, E] = \frac{2}{|\tilde{Q}|} \sum_n \left| \{\mathbf{k} \in \tilde{Q} \,|\, E_n(\mathbf{k}) \leq E\} \right| \tag{176}$$

where $|\tilde{Q}|$ is the Lebesgue measure of $\tilde{Q}$ and $|\{\cdots\}|$ is the Lebesgue measure of $\{\cdots\}$.

We note that since $E_n(\mathbf{k}) \to \infty$ uniformly in $\mathbf{k}$ as $n \to \infty$ (Problem 144), the number $\rho(-\infty, E]$ is finite. Moreover, one can show easily (Problem 145) from our general analysis that ρ is absolutely continuous with respect to dE, Lebesgue measure on $\mathbb{R}$. The Radon–Nikodym derivative $d\rho/dE$ is usually called the **density of states**. To explain the importance of ρ to an analysis of solids, we introduce another notion. Let Q be the basic x-space cell and, given $m \in \mathbb{Z}$, let $Q^{(m)}$ be the set of volume $m^3|Q|$ obtained by stacking up an $m \times m \times m$ set of Q's. Let H_m be the operator $-\Delta_{\mathbf{P}} + V$ on $L^2(Q^{(m)})$ where $-\Delta_{\mathbf{P}}$ denotes periodic boundary conditions. Let $P_m(\Omega)$ be the spectral projections for H_m and define

$$\rho_m(-\infty, E] = 2 \dim P_m(-\infty, E]/m^3$$

Then:

Theorem XIII.101 As $m \to \infty$, $\rho_m \to \rho$ in the sense that $\rho_m(-\infty, E] \to \rho(-\infty, E]$ for every E.

Proof We sketch the main ideas, leaving the details to the reader (Problem 147). The key point is that H_m has a direct *sum* decomposition described as follows. Parametrize $\tilde{Q}$ as $\{\sum_{i=1}^{3} t_i \mathbf{K}_i \,|\, 0 \le t_i < 1\}$. Then

$$L^2(Q^{(m)}) \cong \bigoplus_{\alpha_1, \alpha_2, \alpha_3 = 0}^{m-1} \ell^2(\mathbb{Z}^3)$$

in such a way that H_m becomes

$$\bigoplus_{\alpha_1, \alpha_2, \alpha_3 = 0}^{m-1} H\left(\frac{\alpha_1}{m}\mathbf{K}_1 + \frac{\alpha_2}{m}\mathbf{K}_2 + \frac{\alpha_3}{m}\mathbf{K}_3\right)$$

where $H(\mathbf{k})$ are the fibers of the infinite volume operator H. The reason that this decomposition holds is that one shows that any φ periodic on $Q^{(m)}$ is a sum of φ's with $\varphi(\mathbf{x} + \mathbf{a}_j) = e^{2\pi\alpha_j i/m}\varphi(\mathbf{x})$. As a result of this decomposition,

$$\rho_m(-\infty, E] = 2m^{-3} \#\{n; \alpha_i \in \{0, 1, \ldots, m-1\} \,|\, E_n(m^{-1} \textstyle\sum (\alpha_j \mathbf{K}_j)) \le E\}$$

and, since $E(\cdot)$ is continuous, this expression is an approximation for $\rho(-\infty, E]$. ∎

Now we return to our model of solids. Suppose that each nucleus in free space is surrounded by ℓ electrons. Then in our model we wish to have ℓ electrons per unit cell. While we ignore interactions between the electrons,

we cannot ignore the Pauli principle which asserts for noninteracting electrons that each eigenvalue of H can contain at most two electrons. How do we take this into account when H does not have eigenfunctions and when there are infinitely many electrons (in our infinite crystal lattice!)? We claim that a reasonable way of taking the Pauli principle into account is to say that in the ground state, the electrons fill up the continuum eigenstates up to that energy E where $\rho(-\infty, E] = \ell$. For if we have a large but finite $m \times m \times m$ crystal with periodic boundary conditions, there are $m^3\ell$ electrons, and in the ground state these fill up the eigenstates of H_m to an energy E_m determined by $\rho_m(-\infty, E_m) = \ell$. The smallest number E with $\rho(-\infty, E] = \ell$ is called the **Fermi energy**, E_F. The set of $\mathbf{k} \in B$, the Brillouin zone, with $E_n(\mathbf{k}) = E_F$ for some n is called the **Fermi surface**. This picture is similar to the elementary discussion of the periodic table based on the hydrogen atom but with the complication of continuum states.

We are now in a position to explain why electron conduction is hard in some solids (insulators) and easy in others (metals). In the ground state one can use complex conjugation symmetry to prove that there is no net movement of electrons. To get flow of electrons one must excite some of the electrons. We have seen that typically a periodic Schrödinger operator has gaps in its spectrum. There is a qualitative difference if E_F occurs at the bottom of a gap or not. If E_F is at the bottom of a gap, then H has no spectrum in $(E_F, E_F + \varepsilon)$ and there is a discrete amount of energy needed to

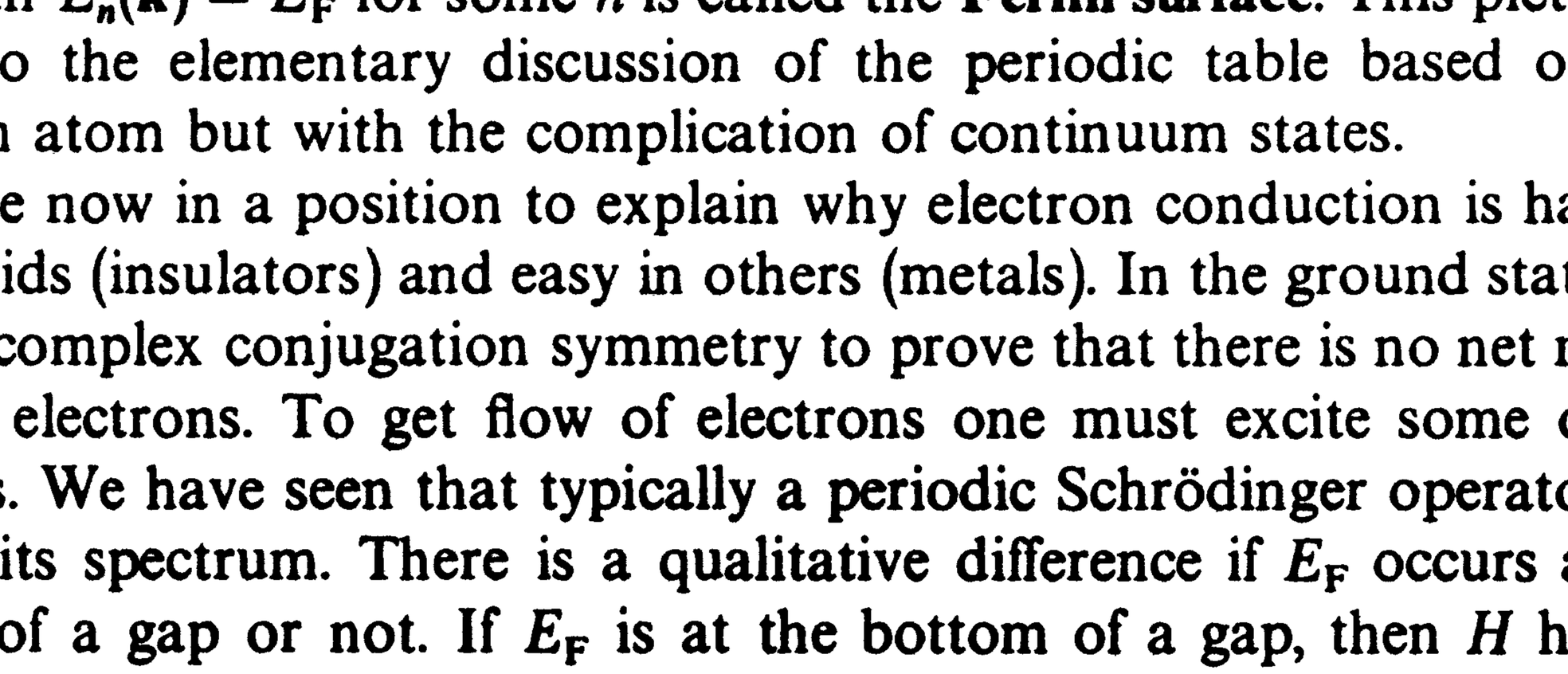


FIGURE XIII.20 Energy bands in conductors and insulators.

set up a current (see Figure XIII.20). In this case one has an insulator. If E_F is not at the bottom of a gap, one has a metal! Of course, if E_F is at the bottom of a small gap (ε small) or if E_F is not at the bottom of a gap but is fairly close

to the bottom of a gap, then one has an intermediate case where the metal/insulator distinction is not sharp (semimetals, semiconductors) and in dealing with real solids one must take into account the fact that the solid is not in the ground state but rather in a finite temperature state determined by statistical mechanics. Notice that the gaps in the spectrum are crucial for this theory of insulators versus metals.

As a final topic in the one-electron theory of solids, we mention impurity scattering. Suppose that one of the lattice points has an impurity atom instead of the kind of atom at all the other sites. An electron in this crystal experiences a potential $V + W$ where V is periodic and W, which represents the difference of the potential of the impurity and what it replaces, is short range. One expects electrons in such a crystal to scatter from the impurity according to the usual scattering theory formalism.

Theorem XIII.102 Let V be a periodic potential on $\mathbb{R}^3$ that is square integrable over a basic cell. Let W be a potential in $L^1 \cap L^2(\mathbb{R}^3)$. Then

$$\Omega^{\pm} = \text{s-lim}_{t \to \mp\infty} \exp[+it(H_0 + V + W)] \exp[-it(H_0 + V)]$$

exist and have identical ranges and, in particular, the S matrix is unitary.

Proof Since $H_0 + V$ has purely absolutely continuous spectrum (Theorem XIII.100), we can prove the theorem by showing that $(-\Delta + V + W + c)^{-1} - (-\Delta + V + c)^{-1}$ is trace class for some c, for then we can apply the Kato–Birman theory (Theorem XI.9). Choose c so that $-\Delta + V + W \geq -c + 1$, $-\Delta + V \geq -c + 1$. Since V and W are $-\Delta$-bounded with relative bound zero,

$$\begin{aligned}
&(-\Delta + V + W + c)^{-1} - (-\Delta + V + c)^{-1} \\
&\quad = -(-\Delta + V + W + c)^{-1} W (-\Delta + V + c)^{-1} \\
&\quad = -[(-\Delta + V + W + c)^{-1}(-\Delta + 1)][(-\Delta + 1)^{-1} W (-\Delta + 1)^{-1}] \\
&\qquad \times [(-\Delta + 1)(-\Delta + V + c)^{-1}]
\end{aligned}$$

The first and third factors are bounded operators by the relative boundedness and since $W \in L^1 \cap L^2$, the middle factor is trace class (see Theorem XI.20). Thus the difference of resolvents is trace class. ∎

XIII.17 An introduction to the spectral theory of non-self-adjoint operators

Thus far we have been mainly concerned with the spectral analysis of self-adjoint operators. In this final section we wish to say something about the spectral analysis of compact operators that need not be self-adjoint. In Section VI.5 we have already seen that if A is a compact operator, then $\sigma(A)$ consists of zero and a set of nonzero numbers $\{\lambda_i\}_{i=1}^{N(A)}$, where $N(A)$ is finite or countably infinite. Only zero can be an accumulation point. Moreover, each λ_i is an eigenvalue, and, by the analysis of Sections XII.1 and XII.2, each spectral projection

$$P_i = -(2\pi i)^{-1} \int_{|\lambda - \lambda_i| = \varepsilon} (A - \lambda)^{-1}\, d\lambda$$

is finite dimensional and Ran $P_i = \{\psi \,|\, (A - \lambda_i)^n \psi = 0 \text{ for some } n\}$. We call a vector ψ a **generalized eigenvector** if $(A - \lambda)^n \psi = 0$ for some $n \geq 1$. Among the natural questions are:

(1) Do the eigenvectors and generalized eigenvectors of A (vectors in the range of some P_i or solutions of $A^n \psi = 0$ for some n) span $\mathscr{H}$, i.e., are they a total set?

(2) Suppose that A is in the trace class $\mathscr{I}_1$ defined in Section VI.6. Let $\lambda_i(A)$ be a listing of the nonzero eigenvalues of A. Each eigenvalue is repeated a number of times equal to dim P_i, its **algebraic multiplicity**. Is it true that

$$\mathrm{Tr}(A) = \sum_{j=1}^{N(A)} \lambda_j(A) \tag{177}$$

(3) By the meromorphic Fredholm theorem, Theorem XIII.13, $(1 + \mu A)^{-1}$ is a meromorphic function of μ on all of $\mathbb{C}$. Can one find explicit functions, entire in μ, with simple expressions in terms of A so that $(1 + \mu A)^{-1} = F(\mu)/G(\mu)$?

We shall discuss a solution of problem 3 in the case where A is trace class and use this solution to discuss problems 1 and 2. We close the section with a discussion of "explicit" solutions to two integral equations which have arisen previously in Volume I and in this volume. Problem 2 is not as obvious as it seems. In the first place it is not a priori clear that the sum converges. Moreover, if A has only zero as eigenvalue, it is far from obvious

that Tr(A), which is defined as a sum of diagonal matrix elements, is zero. Finally, as regards Problem 1, consider the following example:

Example 1 Let $\{\varphi_n\}_{n=1}^{\infty}$ be an orthonormal basis of $\mathscr{H}$. Let $\{\alpha_n\}_{n=1}^{\infty}$ be a sequence of positive numbers converging monotonically to zero. Let

$$A = \sum_{n=1}^{\infty} \alpha_n(\varphi_n, \cdot)\varphi_{n+1}$$

A is compact since

$$\left\| A - \sum_{n=1}^{N} \alpha_n(\varphi_n, \cdot)\varphi_{n+1} \right\| = \sup_{n \geq N+1} |\alpha_n| \to 0$$

Moreover

$$\|A^n\|^{1/n} = \left(\prod_{m=1}^{n} |\alpha_m| \right)^{1/n}$$

goes to zero as $n \to \infty$. Thus, by the spectral radius formula, Theorem VI.6, $\sigma(A) = \{0\}$. Suppose all $\alpha_n \neq 0$. Since it is then clear that $\mathrm{Ker}(A^n) = \{0\}$, A has no eigenvalues, and the span of the eigenvectors is $\{0\}$.

Example 2 Suppose that $\{\psi_n\}_{n=-\infty}^{\infty}$ is a basis of $\mathscr{H}$ and $\{\alpha_n\}$ is a two-sided sequence of nonzero numbers going to zero at $\pm\infty$. Let

$$A = \sum_{n=-\infty}^{\infty} \alpha_n(\psi_n, \cdot)\psi_{n+1}$$

Then

$$B = A^{-1} \equiv \sum_{n=-\infty}^{\infty} \alpha_n^{-1}(\psi_{n+1}, \cdot)\psi_n$$

is a densely defined operator on

$$D(B) = \{\eta \,|\, \textstyle\sum \alpha_n^{-2} |(\psi_{n+1}, \eta)|^2 < \infty\}$$

Note that since $\sigma(A) = \{0\}$, $(B - \lambda)^{-1} = A(1 - \lambda A)^{-1}$. Thus, B is a closed operator with all of $\mathbb{C}$ as its resolvent set! (See also Example 5 in Section VIII.1.)

Thus, problem 1 does not have an affirmative answer in all cases. Later, we shall show that if A is a strictly m-accretive operator that is trace class, then its generalized eigenvectors span $\mathscr{H}$.

Henceforth, $\{\lambda_n(A)\}_{n=1}^{N(A)}$ will be a listing of all nonzero eigenvalues of A, a compact operator. Each eigenvalue appears a number of times equal to its algebraic multiplicity. We order them by requiring that $|\lambda_{n+1}(A)| \leq |\lambda_n(A)|$ and $\arg \lambda_{n+1}(A) \geq \arg \lambda_n(A)$ if $|\lambda_{n+1}(A)| = |\lambda_n(A)|$ where $\arg \lambda_i \in [0, 2\pi)$. As a preliminary, we shall prove that the sum $\sum_{n=1}^{N(A)} \lambda_n(A)$ converges absolutely if $A \in \mathscr{I}_1$.

Lemma 1 Let A be any compact operator. Then there exists an orthonormal set $\{e_n\}_{n=1}^{N(A)}$, so that

$$Ae_n = \lambda_n(A)e_n + \sum_{m=1}^{n-1} v_{nm}\, e_m \tag{178}$$

for suitable v_{nm}. In particular,

$$(e_n\,,\, Ae_n) = \lambda_n(A) \tag{179}$$

Proof Let P_i be the spectral projections for nonzero eigenvalues. By writing a Jordan normal form for $A \restriction \operatorname{Ran} P_i$ for each i, we can find a set of algebraically independent vectors, $\{f_j\}_{j=1}^{N(A)}$ so that

$$Af_n = \lambda_n(A)f_n + \beta_n\, f_{n-1} \tag{180}$$

where β_n is either 1 or 0. By applying a Gram–Schmidt procedure to $\{f_n\}_{n=1}^{N(A)}$, we find an orthonormal set $\{e_n\}_{n=1}^{N(A)}$ so that

$$e_n = \sum_{m=1}^{n} \gamma_{nm}\, f_m \tag{181}$$

with $\gamma_{nn} \neq 0$. (178) follows from (180) and (181). ∎

The orthonormal set $\{e_n\}_{n=1}^{N(A)}$ is called a **Schur basis** (although it need not be a basis!).

Now let $\{\mu_n(A)\}$ be the singular values of A, i.e., the eigenvalues of $|A|$.

Theorem XIII.103 (Schur–Lalesco–Weyl theorem) For any $1 \leq p < \infty$,

$$\sum_{n=1}^{N(A)} |\lambda_n(A)|^p \leq \sum_{n=1}^{\infty} \mu_n(A)^p \tag{182}$$

where A is compact, $\{\lambda_n(A)\}$ are its eigenvalues, and $\{\mu_n(A)\}$ its singular values. In particular, if $A \in \mathscr{I}_1$,

$$\sum_{n=1}^{N(A)} |\lambda_n(A)| < \infty$$

Proof Consider the canonical expansion for A

$$A = \sum_{n=1}^{\infty} \mu_n(A)(f_n, \cdot)g_n$$

where $\{f_n\}$ and $\{g_n\}$ are orthonormal sets (Theorem VI.17). Let $\{e_n\}_{n=1}^{N(A)}$ be a Schur basis for A. Then, by (179),

$$\lambda_m(A) = \sum_{n=1}^{\infty} \alpha_{mn}\mu_n(A)$$

where

$$\alpha_{mn} = (f_n, e_m)(e_m, g_n)$$

Now, we claim that

$$\sum_{n=1}^{\infty} |\alpha_{mn}| \leq 1 \tag{183}$$

$$\sum_{m=1}^{\infty} |\alpha_{mn}| \leq 1 \tag{184}$$

To prove (184), note that by the Schwarz inequality,

$$\begin{aligned}\sum_{m=1}^{\infty} |\alpha_{mn}| &\leq \left(\sum_{m=1}^{\infty} |(f_n, e_m)|^2\right)^{1/2}\left(\sum_{m=1}^{\infty} |(g_n, e_m)|^2\right)^{1/2} \\ &\leq \|f_n\| \, \|g_n\| = 1\end{aligned}$$

where we have used Bessel's inequality in the last step together with the fact that $\{e_m\}$ is an orthonormal set. (183) follows similarly using the fact that $\{g_n\}$ and $\{f_n\}$ are orthonormal sets. Now, let q be the dual index to p. Then

$$\begin{aligned}\sum_{m=1}^{M} |\lambda_m(A)|^p &\leq \sum_{m=1}^{M} |\lambda_m(A)|^{p-1} \sum_{n=1}^{\infty} |\alpha_{mn}| \, |\mu_n(A)| \\ &= \sum_{n,m} |\alpha_{nm}|^{1/p} |\alpha_{nm}|^{1/q} |\lambda_m|^{p-1} |\mu_n| \\ &\leq \left(\sum_{n,m} |\alpha_{nm}| \, |\mu_n|^p\right)^{1/p}\left(\sum_{n,m} |\alpha_{nm}| \, |\lambda_m|^p\right)^{1/q} \\ &\leq \left(\sum_{n} |\mu_n|^p\right)^{1/p}\left(\sum_{m=1}^{M} |\lambda_m|^p\right)^{1/q}\end{aligned}$$

In the next to the last step, we have used Hölder's inequality and the fact that $q(p-1) = p$. In the last step we used (183) and (184). (182) now follows easily. ∎

Before turning to the main topic of this section, we note one consequence of (182).

Corollary (generalized Golden–Thompson inequality) Let $-A$ and $-B$ be positive self-adjoint operators with $A + B$ essentially self-adjoint on $D(A) \cap D(B)$. Suppose that $e^{A/2}e^{B}e^{A/2} \in \mathscr{I}_p$. Then $e^{A+B} \in \mathscr{I}_p$ and

$$\|e^{A+B}\|_p \leq \|e^{A/2}e^{B}e^{A/2}\|_p$$

Proof We first prove that if C and D are bounded positive operators and $CD \in \mathscr{I}_r$, then $C^{1/2}DC^{1/2} \in \mathscr{I}_r$ and

$$\|C^{1/2}DC^{1/2}\|_r \leq \|CD\|_r$$

First note that for any bounded E, F, we have $\sigma(EF)\backslash\{0\} = \sigma(FE)\backslash\{0\}$ (Problem 166a) and if $\lambda \neq 0$ is an eigenvalue of EF it is an eigenvalue of FE with the same multiplicity (Problem 166b). Since $CD = C^{1/2}(C^{1/2}D) \in \mathscr{I}_r$, it has purely discrete spectrum away from 0, so the self-adjoint operator $C^{1/2}DC^{1/2}$ has purely discrete spectrum away from zero and thus, is a compact operator. By the above, $\lambda_n(C^{1/2}DC^{1/2}) = \lambda_n(CD)$ and since $C^{1/2}DC^{1/2}$ is self-adjoint and positive, $\lambda_n(C^{1/2}DC^{1/2}) = \mu_n(C^{1/2}DC^{1/2})$. Thus, using (182),

$$\begin{aligned}\|C^{1/2}DC^{1/2}\|_r^r &= \sum_n |\lambda_n(CD)|^r \\ &\leq \sum_n |\mu_n(CD)|^r = \|CD\|_r^r\end{aligned}$$

Now we claim that $Q_n = (e^{A/2^{n+1}}e^{B/2^n}e^{A/2^{n+1}})^{2^n} \in \mathscr{I}_p$ with

$$\|Q_n\|_p \leq \|e^{A/2}e^{B}e^{A/2}\|_p$$

We prove this inductively. $n = 0$ is trivial. Let $C_n = e^{A/2^n}$, $D_n = e^{B/2^n}$ and let $r_n = 2^n p$. Then if $Q_{n-1} \in \mathscr{I}_p$, $C_n D_n \in \mathscr{I}_{r_n}$ and

$$\|Q_n\|_p = \|C_n^{1/2}D_nC_n^{1/2}\|_{r_n}^{2^n} \leq \|C_nD_n\|_{r_n}^{2^n} = \|Q_{n-1}\|_p$$

proving the bound on $\|Q_n\|_p$ inductively.

By the Trotter product formula, $Q_n \to e^{A+B}$ strongly so that (Problem 167) $e^{A+B} \in \mathscr{I}_p$ and

$$\|e^{A+B}\|_p \leq \overline{\lim}\|Q_n\|_p \leq \|e^{A/2}e^{B}e^{A/2}\|_p \quad \blacksquare$$

Our first goal will be a proof of (177). In proving this we shall develop a theory of infinite determinants which is useful in other contexts. These determinants will depend on our development of a little alternating algebra, i.e., the theory of antisymmetric tensor products. In Sections II.4 and VIII.10 we

presented the basic definition of these objects as "Fermion Fock spaces," but we repeat the definition here with slightly different notation. Given a Hilbert space $\mathscr{H}$, $\bigotimes^n\mathscr{H}$ is defined as the vector space of multilinear functionals on $\mathscr{H}$. Explicitly, given $\varphi_1, \ldots, \varphi_n \in \mathscr{H}$, we define $\varphi_1 \otimes \cdots \otimes \varphi_n \in \bigotimes^n\mathscr{H}$ by

$$(\varphi_1 \otimes \cdots \otimes \varphi_n)(\langle \eta_1, \ldots, \eta_n \rangle) = (\varphi_1, \eta_1) \cdots (\varphi_n, \eta_n)$$

One can show (see Proposition 1 in Section II.4) that the finite span of the $\{\varphi_1 \otimes \cdots \otimes \varphi_n\}$ possesses a well-defined inner product with

$$((\varphi_1 \otimes \cdots \otimes \varphi_n), (\eta_1 \otimes \cdots \otimes \eta_n)) = (\varphi_1, \eta_1) \cdots (\varphi_n, \eta_n)$$

$\bigotimes^n\mathscr{H}$ is the completion of this finite span in the topology generated by this inner product. Given any $A \in \mathscr{L}(\mathscr{H})$, there is a natural operator $\Gamma_n(A)$ in $\mathscr{L}(\bigotimes^n\mathscr{H})$ with

$$\Gamma_n(A)(\varphi_1 \otimes \cdots \otimes \varphi_n) = A\varphi_1 \otimes \cdots \otimes A\varphi_n$$

Γ_n is a functor, that is, $\Gamma_n(AB) = \Gamma_n(A)\Gamma_n(B)$.

Let $\mathscr{P}_n$ denote the group of all permutations on n letters. Let $\varepsilon(\cdot)$ be the function on $\mathscr{P}_n$ that is $+1$ (respectively, -1) on even (respectively, odd) permutations. Define $\varphi_1 \wedge \cdots \wedge \varphi_n \in \bigotimes^n\mathscr{H}$ by

$$\varphi_1 \wedge \cdots \wedge \varphi_n = (n!)^{-1/2} \sum_{\pi \in \mathscr{P}_n} \varepsilon(\pi)[\varphi_{\pi(1)} \otimes \cdots \otimes \varphi_{\pi(n)}] \tag{185}$$

and define $\bigwedge^n(\mathscr{H})$ to be the subspace of $\bigotimes^n\mathscr{H}$ spanned by the $\{\varphi_1 \wedge \cdots \wedge \varphi_n\}$. The $(n!)^{-1/2}$ normalization factor is chosen so that if $\varphi_1, \ldots, \varphi_n$ are orthornormal, then $\varphi_1 \wedge \cdots \wedge \varphi_n$ has norm one. More generally, from (185) one can see that (Problem 149)

$$(\varphi_1 \wedge \cdots \wedge \varphi_n, \eta_1 \wedge \cdots \wedge \eta_n) = \det((\varphi_i, \eta_j)) \tag{186}$$

where $\det(a_{ij}) = \sum_{\pi \in \mathscr{P}_n} \varepsilon(\pi) a_{1\pi(1)} \cdots a_{n\pi(n)}$.

Given $A \in \mathscr{L}(\mathscr{H})$, $\Gamma_n(A)$ leaves $\bigwedge^n\mathscr{H}$ invariant, and we denote its restriction to $\bigwedge^n\mathscr{H}$ by $\bigwedge^n(A)$. Since Γ_n is a functor, so is $\bigwedge^n$.

$$\bigwedge^n(AB) = \bigwedge^n(A)\bigwedge^n(B) \tag{187}$$

When $n = 0$, we define $\bigwedge^n\mathscr{H}$ to be $\mathbb{C}$ and $\bigwedge^n(A)$ as $1 : \mathbb{C} \to \mathbb{C}$.

The connection between determinants of finite-dimensional operators and $\bigwedge^n(\cdot)$ is given by:

Lemma 2

(a) Let $\mathscr{H}$ be an n-dimensional Hilbert space. Then $\bigwedge^n\mathscr{H}$ is one dimensional.

(b) If $\mathscr{H}$ has dimension n, then $\bigwedge^n(A)$ is multiplication by the number $\det(A)$, the ordinary determinant of A.
(c) $\det(AB) = \det(A)\det(B)$.

Proof (a) We shall show more generally that $\dim \bigwedge^k \mathscr{H} = \binom{n}{k}$, the number of ways of choosing k objects from among n objects. For let $e_1, \ldots, e_n$ be an orthonormal basis for $\mathscr{H}$. We claim that

$$\{e_{i_1} \wedge \cdots \wedge e_{i_k} | 1 \leq i_1 < i_2 < \cdots < i_k \leq n\}$$

is an orthonormal basis for $\bigwedge^k \mathscr{H}$; this proves $\dim \bigwedge^k \mathscr{H} = \binom{n}{k}$. For the vectors in question are orthonormal and so independent, and they span $\bigwedge^k \mathscr{H}$ since $\langle \varphi_1, \ldots, \varphi_k \rangle \to \varphi_1 \wedge \cdots \wedge \varphi_k$ is multilinear and antisymmetric under interchanges.

(b) Since $\bigwedge^n(\mathscr{H})$ is one dimensional, $\bigwedge^n(A)$ must be multiplication by some number α. If $e_1, \ldots, e_n$ is an orthonormal basis, then

$$\begin{aligned} \alpha &= (e_1 \wedge \cdots \wedge e_n, \bigwedge^n(A)(e_1 \wedge \cdots \wedge e_n)) \\ &= (e_1 \wedge \cdots \wedge e_n, Ae_1 \wedge \cdots \wedge Ae_n) \\ &= \det((e_i, Ae_j)) \end{aligned}$$

by (186).

(c) follows from (b) and (187). ∎

This rather effortless proof of $\det(AB) = \det(A)\det(B)$ shows the power of alternating algebra in studying determinants.

To understand the definition that we shall take for $\det(1 + A)$ when $A \in \mathscr{I}_1$, suppose that A is an operator on a finite-dimensional space $\mathscr{H}$ with $\dim \mathscr{H} = n$. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A and let $e_1, \ldots, e_n$ be a Schur basis for A. Then, it is easy to see that

$$\det(1 + A) = (e_1 \wedge \cdots \wedge e_n, (1 + A)e_1 \wedge \cdots \wedge (1 + A)e_n) = \prod_{j=1}^{n} (1 + \lambda_i)$$

and

$$\begin{aligned} \operatorname{Tr}(\bigwedge^k(A)) &= \sum_{1 \leq i_1 < \cdots < i_k \leq n} ((e_{i_1} \wedge \cdots \wedge e_{i_k}), (Ae_{i_1} \wedge \cdots \wedge Ae_{i_k})) \\ &= \sum_{1 \leq i_1 \cdots \leq n} \lambda_{i_1} \cdots \lambda_{i_k} \end{aligned}$$

so that

$$\det(1 + A) = \sum_{j=0}^{n} \operatorname{Tr}(\bigwedge^j(A)) \tag{188}$$

in case dim $\mathscr{H} = n$. In the case dim $\mathscr{H} = \infty$, we shall *define* $\det(1 + A)$ by (188). To prove that the sum converges, we need the following lemma:

Lemma 3 Let A be a trace class operator with singular values $\mu_n(A)$. Then, for any k, $\bigwedge^k(A)$ is trace class and

(a) $$\|\bigwedge^k(A)\|_1 = \sum_{i_1 < \cdots < i_k} \mu_{i_1}(A) \cdots \mu_{i_k}(A)$$

(b) $$\|\bigwedge^k(A)\|_1 \leq \|A\|_1^k / k!$$

Proof Let $A = U|A|$ be the polar decomposition for A (Theorem VI.10). It is easy to see that $\bigwedge^k(A) = \bigwedge^k(U)\bigwedge^k(|A|)$ is the polar decomposition for $\bigwedge^k(A)$ and in particular that

$$|\bigwedge^k(A)| = \bigwedge^k(|A|)$$

Let $e_1, \ldots$ be the orthonormal basis of eigenvectors for $|A|$. Then $e_{i_1} \wedge \cdots \wedge e_{i_k}$ are an orthonormal basis of eigenvectors for $\bigwedge^k(|A|)$. Thus

$$\begin{aligned} \operatorname{Tr}(|\bigwedge^k(A)|) &= \sum_{i_1 < \cdots < i_k} \mu_{i_1}(A) \cdots \mu_{i_k}(A) \\ &\leq \frac{1}{k!} \sum_{i_1, \ldots, i_k} \mu_{i_1}(A) \cdots \mu_{i_k}(A) \\ &= [\operatorname{Tr}(|A|)]^k / k! \end{aligned}$$

Thus $\bigwedge^k(A)$ is trace class and (a) and (b) hold. ∎

Definition Let $A \in \mathscr{I}_1$. Then $\det(1 + A)$ is defined by

$$\det(1 + A) = \sum_{k=0}^{\infty} \operatorname{Tr}(\bigwedge^k(A)) \tag{188}$$

Lemma 4 The sum (188) converges for each $A \in \mathscr{I}_1$. Moreover:

(a) $|\det(1 + A)| \leq \prod_{j=1}^{\infty} (1 + \mu_j(A))$.
(b) $|\det(1 + A)| \leq \exp(\|A\|_1)$.
(c) For any $A_1, \ldots, A_n \in \mathscr{I}_1$,

$$\langle z_1, \ldots, z_n \rangle \to \det\left(1 + \sum_{i=1}^{n} z_i A_i\right)$$

is an entire analytic function.

(d) For any $A, B \in \mathscr{I}_1$

$$|\det(1 + A) - \det(1 + B)| \leq \|A - B\|_1 \exp(\|A\|_1 + \|B\|_1 + 1) \tag{189}$$

Proof Since $|\mathrm{Tr}(\bigwedge^k(A))| \leq \|\bigwedge^k(A)\|_1/k!$, the convergence of (188) and (a) and (b) follow from Lemma 3. Since we have estimates on the terms of (188) that are uniform on compact sets in $\mathbb{C}^n$, it is sufficient to prove that

$$\langle z_1, \ldots, z_n \rangle \to \mathrm{Tr}(\bigwedge^k(z_1 A_1 + \cdots + z_k A_k))$$

is analytic. Clearly, $\bigwedge^k(z_1 A_1 + \cdots + z_k A)$ is analytic as an $\mathscr{I}_1$-valued function, so its trace is analytic for $\mathrm{Tr}(\cdot)$ is a bounded linear functional on $\mathscr{I}_1$. This proves (c). (d) follows from (b) and (c) and the theorem immediately below. ∎

Theorem XIII.104 Let X be a complex Banach space. Let $F: X \to \mathbb{C}$ be a function with the following properties:

(i) For any $x, y \in X$, $\mu \to F(x + \mu y)$ is an entire function of μ.

(ii) For some monotone increasing function G on $[0, \infty)$,

$$|F(x)| \leq G(\|x\|)$$

for all $x \in X$.

Then

$$|F(x) - F(y)| \leq \|x - y\| G(\|x\| + \|y\| + 1) \tag{190}$$

Proof Fix x and y in X and let $f: \mathbb{C} \to \mathbb{C}$ be given by

$$f(\mu) = F(\tfrac{1}{2}(x + y) + \mu(y - x))$$

so that f is an entire function by (a). Notice that

$$|F(x) - F(y)| = |f(-\tfrac{1}{2}) - f(\tfrac{1}{2})| \leq \sup_{-1/2 \leq t \leq 1/2} |f'(t)| \tag{191}$$

Now, by the Cauchy integral formula,

$$f'(t) = (2\pi i)^{-1} \oint_{|\mu - t| = \|x - y\|^{-1}} \frac{f(\mu)\, d\mu}{(\mu - t)^2}$$

so that

$$\sup_{|t| \leq 1/2} |f'(t)| \leq \|x - y\| \sup_{|\mu| \leq 1/2 + \|x - y\|^{-1}} |f(\mu)| \tag{192}$$

For $|\mu| \leq \frac{1}{2} + \|x - y\|^{-1}$, we have that

$$\|\tfrac{1}{2}(x + y) + \mu(y - x)\| \leq \|x\| + \|y\| + 1$$

so, for such μ,

$$|f(\mu)| \leq G(\|x\| + \|y\| + 1) \tag{193}$$

by (ii). (191)–(193) imply (190). ∎

Suppose that $A \in \mathscr{I}_1$. The idea in proving that $\mathrm{Tr}(A) = \sum \lambda_n(A)$ is the following: Suppose that we can prove that $\det(1 + zA)$ has the convergent expansion $\prod_{j=1}^{N(A)} (1 + z\lambda_j(A))$. The term linear in z in the product is clearly $\sum_{j=1}^{N(A)} \lambda_j(A)$ while the linear term in $\det(1 + zA)$ is by definition $\mathrm{Tr}(A)$. Thus, we want to study the function $\det(1 + zA)$. We first summarize the properties of $\det(1 + A)$.

Theorem XIII.105 Let A and B be in $\mathscr{I}_1$. Then:

(a) $\det(1 + A)\det(1 + B) = \det(1 + A + B + AB)$. (194)
(b) $(1 + A)$ is invertible if and only if $\det(1 + A) \neq 0$.
(c) If $-\mu^{-1}$ is an eigenvalue of A, then $\det(1 + zA)$ has a zero of order n at $z = \mu$ where n is the algebraic multiplicity of $-\mu^{-1}$.
(d) For any ε, there is a C_ε, depending on A, so that

$$|\det(1 + zA)| \leq C_\varepsilon \exp(\varepsilon|z|)$$

Proof (a) Since the finite rank operators are dense in $\mathscr{I}_1$ (corollary to Theorem VI.21) and $\det(1 + \cdot)$ is continuous by (189), we need only verify (194) for finite rank A and B. Let V be the span of $\mathrm{Ker}(A)^\perp$, $\mathrm{Ker}(B)^\perp$, Ran A, and Ran B. Then V is finite dimensional, invariant under A, B, A^*, and B^*, and A and B are zero on $V^\perp$. Thus A and B leave V and $V^\perp$ invariant. Let $\tilde{A} = A \restriction V$, $\tilde{B} = B \restriction V$. Then $\mathrm{Tr}(\bigwedge^k(A)) = \mathrm{Tr}(\bigwedge^k(\tilde{A}))$, etc. Therefore,

$$\det(1 + A) = \det_V(1 + \tilde{A})$$

and similarly for B, and $A + B + AB$, where $\det_V$ is the determinant on V. (194) now follows from the finite-dimensional result, Lemma 2c.

(b) If $1 + A$ is invertible, then $(1 + A)^{-1} = 1 + B$ with $B = -A(1 + A)^{-1} \in \mathscr{I}_1$. Thus, by (194),

$$\det(1 + A)\det(1 + B) = \det(1) = 1$$

so $\det(1 + A) \neq 0$. If $1 + A$ is not invertible, then -1 is an eigenvalue of A, so $\det(1 + A) = 0$ by the result (c) that we are about to prove.

(c) Let P be the spectral projection of $-\mu^{-1}$. Let $B = AP$ and $C = A(1-P)$. Then

$$1 + zA = (1 + zB)(1 + zC)$$

so $\det(1 + zA) = \det(1 + zB)\det(1 + zC)$. Since $1 + zC$ is invertible for z near $-\mu^{-1}$, it suffices to show that $\det(1 + zB)$ has an nth-order zero at $-\mu^{-1}$. By extending a Schur basis for B to a basis for $\mathscr{H}$, we can find an orthonormal basis, with

$$Be_i = \lambda_i e_i + \sum_{j=1}^{i-1} \alpha_{ij} e_j$$

with $\lambda_1 = \cdots = \lambda_n = -\mu^{-1}$ and $\lambda_{n+1} = \cdots = 0$. We just use the fact that Ran $B \subset P =$ span of the Schur basis. It follows easily that $\operatorname{Tr}(\bigwedge^k(B)) = \binom{n}{k}(-\mu^{-1})^k$ for $k \leq n$ and $\operatorname{Tr}(\bigwedge^k(B)) = 0$ if $k > n$. Thus, $\det(1 + zB) = (1 - z\mu^{-1})^n$ has an nth-order zero at $z = \mu$.

(d) Let $\mu_n(A)$ be the singular values of A. Choose N so that

$$\sum_{n>N} \mu_n(A) < \varepsilon/2$$

Then, by Lemma 4a,

$$\begin{aligned} |\det(1 + zA)| &\leq \prod_{j=1}^{\infty} (1 + |z|\mu_j(A)) \\ &\leq \prod_{j=1}^{N} (1 + |z|\mu_j(A)) \exp(\tfrac{1}{2}\varepsilon|z|) \end{aligned}$$

since $1 + x \leq e^x$ for $x \geq 0$. Now, since $\prod_{j=1}^{N} (1 + |z|\mu_j(A))$ is a polynomial, we can find C_ε with

$$\prod_{j=1}^{N} (1 + |z|\mu_j(A)) \leq C_\varepsilon \exp(\tfrac{1}{2}\varepsilon|z|) \quad \blacksquare$$

Theorem XIII.106 For any $A \in \mathscr{I}_1$,

$$\det(1 + A) = \prod_{j=1}^{N(A)} (1 + \lambda_j(A))$$

where $\{\lambda_j(A)\}_{j=1}^{N(A)}$ are the eigenvalues of A counted with algebraic multiplicity.

Proof Let $f(z) = \det(1 + zA)$. Let

$$g(z) = \prod_{j=1}^{N(A)} (1 + z\lambda_j(A))$$

If $N(A) = \infty$, the product in question converges to an analytic function by standard results (see Problem 150) because

$$\sum_{j=1}^{\infty} |\lambda_j(A)| < \infty$$

by Theorem XIII.103. We will show that $f(z) = g(z)$. By (b) and (c) of Theorem XIII.105, f and g have the same zeros including order, so f/g is an entire nonvanishing analytic function. Thus,

$$f = ge^h$$

where the ambiguity in h is determined by requiring that h be entire with $h(0) = 0$. This is possible since $f(0) = g(0) = 1$. We shall show that $h(z) = 0$ for $|z| < 1$, so h will be identically zero. For $R \geq 2$, and $|z| < R$ define

$$h_R(z) = \ln[f_R(z)]$$

$$k_R(z) = -\sum_{\{j \mid |\lambda_j|^{-1} > R\}} \ln(1 + z\lambda_j(A))$$

$$f_R(z) = f(z) \Big/ \prod_{\{j \mid |\lambda_j|^{-1} \leq R\}} (1 + z\lambda_j)$$

The ambiguities in h_R and k_R are determined by setting $h_R(0) = k_R(0) = 0$. Notice also that f_R is an entire function. Since $h = h_R + k_R$, it suffices to show that $|h_R(z)| \to 0$ and $|k_R(z)| \to 0$ as $R \to \infty$ for each z with $|z| \leq 1$.

Since $\ln(1 + x)$ vanishes at $x = 0$ and is analytic in a neighborhood of $\{x \mid |x| \leq \frac{1}{2}\}$, we have

$$|\ln(1 + x)| \leq C|x|$$

for suitable C and all x with $|x| \leq \frac{1}{2}$. Thus, for $R \geq 2$,

$$|k_R(z)| \leq |z| \sum_{\{j \mid |\lambda_j|^{-1} > R\}} |\lambda_j(A)| \to 0$$

as $R \to \infty$ since the infinite sum is convergent.

Next, consider the entire function $f_R(z)$. If $|z| = 2R$, and $|\lambda_j|^{-1} \leq R$, then $|1 + z\lambda_j| \geq 1$. Thus, if $|z| = 2R$, $|f_R(z)| \leq C_\varepsilon \exp(2\varepsilon R)$ by (d) of Theorem XIII.105. By the maximum modulus principle, this remains true if $|z| = R$, so

$$\mathrm{Re}(h_R(z)) \leq \ln C_\varepsilon + 2\varepsilon R$$

for $|z| = R$. We shall prove below a lemma that asserts that, for any function analytic in a neighborhood of $|z| \leq R$,

$$\max_{|z|\leq r} |f(z)| \leq \frac{2r}{R-r} \max_{|z|=R} [\mathrm{Re}(f(z))] + \frac{R+r}{R-r} |f(0)|$$

So, since $h_R(0) = 0$,

$$\max_{|z|\leq 1} |h_R(z)| \leq 2(R-1)^{-1}[\ln C_\varepsilon + 2\varepsilon R]$$

Thus, for any z with $|z| \leq 1$,

$$\overline{\lim_{R\to\infty}} |h_R(z)| \leq 4\varepsilon$$

Since ε is arbitrary, $|h_R(z)| \to 0$ as $R \to \infty$. This proves the theorem. ∎

Corollary (Lidskii's theorem) For any $A \in \mathscr{I}_1$

$$\mathrm{Tr}(A) = \sum_{j=1}^{N(A)} \lambda_j(A) \tag{177}$$

where $\lambda_j(A)$ are the eigenvalues of A.

Proof Consider the Taylor expansion for $\det(1 + \mu A)$ about $\mu = 0$. By (188), the first term in the expansion defining det is $\mathrm{Tr}(A)$. The first term in $\prod_{j=1}^{N(A)} (1 + \mu\lambda_j(A))$ is clearly $\sum_{j=1}^{N(A)} \lambda_j(A)$. ∎

One might expect to learn something from each term in the Taylor expansion for $\det(1 + \mu A)$, but the kth term in the series is just (177) for $\bigwedge^k(A)$, i.e.,

$$\mathrm{Tr}(\bigwedge^k(A)) = \sum_{j=1}^{N(\bigwedge^k(A))} \lambda_j(\bigwedge^k(A)) = \sum_{1\leq j_1<\cdots<j_k\leq N(A)} \lambda_{j_1}(A)\cdots\lambda_{j_k}(A)$$

Because of this, one can deduce Theorem XIII.106 from (177).

In our proof of Theorem XIII.106, we used the following fact from complex analysis:

Lemma 5 (Borel–Carathéodory theorem) Let f be analytic in a neighborhood of $|z| \leq R$. Then for any $r < R$,

$$\max_{|z|\leq r} |f(z)| = \frac{2r}{R-r} \max_{|z|=R} [\mathrm{Re}(f(z))] + \frac{R+r}{R-r} |f(0)| \tag{195}$$

Proof We first claim that one can suppose that $f(0) = 0$. For if (195) holds for $h(z) = f(z) - f(0)$, it is easily seen to hold for f. Thus, suppose that $f(0) = 0$ and let $A = \max_{|x|=R}[\mathrm{Re} f(z)]$. Also, without loss suppose that f is not identically zero, so that $A > 0$. By the maximum modulus principle applied to e^f, $\mathrm{Re} f(z) \leq A$ for all z with $|z| \leq R$, so that

$$g(z) \equiv \frac{f(z)}{z(2A - f(z))}$$

is analytic for $|z| < R$. Writing $f = u + iv$, we see that if $|z| = R$,

$$|g(z)|^2 = \frac{1}{R^2} \frac{u^2 + v^2}{(2A - u)^2 + v^2} \leq \frac{1}{R^2}$$

since $|u| \leq |2A - u|$. Thus $|g(z)| \leq 1/R$ for all z with $|z| \leq R$ by the maximum modulus principle. Since

$$f(z) = \frac{2Azg(z)}{1 + zg(z)}$$

we see that, for $|z| = r$,

$$|f(z)| \leq \frac{2Ar/R}{1 - r/R} = \frac{2Ar}{R - r}$$

Again invoking the maximum modulus principle, we conclude that (195) holds. ∎

Next, we use the determinant theory that we have developed to investigate the third question, i.e., to find explicit functions $f(\mu)$ and $g(\mu)$ so that $(1 + \mu A)^{-1} = f(\mu)/g(\mu)$,

Theorem XIII.107 Let $A \in \mathscr{I}_1$. The function

$$F_A(\mu) = [\det(1 + \mu A)][1 + \mu A]^{-1}$$

defined on $\{\mu \mid -\mu^{-1} \notin \sigma(A)\}$ may be extended to all of $\mathbb{C}$ in such a way that F is an entire function. Moreover,

$$\|F_A(\mu)\| \leq \exp(|\mu| \|A\|_1) \tag{196}$$

and

$$\|F_A(1) - F_B(1)\| \leq \|A - B\|_1 \exp(\|A\|_1 + \|B\|_1 + 1) \tag{197}$$

Proof The function $G(\mu) = (1 + \mu A)^{-1}$ is analytic on $\{\mu \mid -\mu^{-1} \notin \sigma(A)\}$ by Theorem VI.5. If we can show that for $-\mu_0^{-1} \in \sigma(A)$, $G(\mu)$ has a pole of order k at $\mu = \mu_0$ where k is less than or equal to the algebraic multiplicity of $-\mu_0^{-1}$, then $\det(1 + \mu A)G(\mu)$ will be regular at $\mu = \mu_0$ since $\det(1 + \mu A)$ has a zero of order equal to that multiplicity. Given such a μ_0, let P be the spectral projection associated to $-\mu_0^{-1}$. Let $B = AP$ and $C = A - B$. Then

$$(1 + \mu A)^{-1} = (1 + \mu B)^{-1}P + (1 + \mu C)^{-1}(1 - P)$$

The second term on the right-hand side is nonsingular at μ_0 since $-\mu_0^{-1} \notin \sigma(C)$. Since B is a finite rank operator, we can explicitly invert $1 + \mu B$ by using the theory of finite-dimensional determinants and cofactor matrices. This realizes $(1 + \mu B)^{-1}$ as a quotient whose denominator $\det(1 + \mu B)$ is a polynomial of degree d where $d = \dim P$. Thus, $(1 + \mu B)^{-1}$ has a pole of order at most d.

It remains to prove (196) and (197). By a simple limiting argument (Problem 151), it suffices to prove (196) in the finite-dimensional case when, in addition, $1 + \mu A$ is invertible. Since $1 + \mu A = U\,|1 + \mu A|$ with U unitary we have

$$\|(1 + \mu A)^{-1} \det(1 + \mu A)\| = \|\,|1 + \mu A|^{-1} \det(|1 + \mu A|)\|$$

Let $\lambda_1, \ldots, \lambda_k$ be the eigenvalues of $|1 + \mu A|$ with $\lambda_1 \geq \cdots \geq \lambda_k$. Then

$$\|\,|1 + \mu A|^{-1} \det(|1 + \mu A|)\| = \lambda_k^{-1}\left[\prod_{i=1}^{k} \lambda_i\right] = \prod_{i=1}^{k-1} \lambda_i$$

Let $\alpha_1, \ldots, \alpha_k$ be the eigenvalues of $|A|$. One can show (Problem 158) that $\lambda_i \leq 1 + |\mu|\alpha_i$. Thus

$$\begin{aligned}\|(1 + \mu A)^{-1} \det(1 + \mu A)\| &\leq \prod_{i=1}^{k-1} (1 + |\mu|\alpha_i) \\ &\leq \prod_{i=1}^{k-1} \exp(|\mu|\alpha_i) \leq \exp(|\mu| \operatorname{Tr} |A|)\end{aligned}$$

This proves (196). (197) now follows from (196) and Theorem XIII.104 applied to the functions $(\varphi, F_A(1)\psi)$ (Problem 170). ∎

One point of the estimates (196) and Lemma 4b is that they allow one to estimate errors made in truncating the power series expansions of $\det(1 + \mu A)$ and $(1 + \mu A)^{-1} \det(1 + \mu A)$. (Problem 152). It is therefore of

interest to find their Taylor coefficients. We already have an expansion of $\det(1 + \mu A)$ in terms of $\bigwedge^k(A)$ and a similar expansion is possible for the function

$$D_\mu(A) \equiv A(1 + \mu A)^{-1} \det(1 + \mu A)$$

in terms of partial traces of $\bigwedge^k(A)$ (Problem 153). This expansion is essentially an abstraction of an expansion used by Fredholm in his famous paper on integral equations. Notice that $D_\mu(A)$ is defined so that

$$(1 + \mu A)^{-1} = 1 - \mu[D_\mu(A)/\det(1 + \mu A)]$$

It is not especially easy to compute $\bigwedge^k(A)$ in terms of A, so that one would like expressions for the Taylor coefficients of $\det(1 + \mu A)$ and $D_\mu(A)$ in terms of quantities like A, A^2, ... and their traces.

Lemma 6 Let A be a fixed element in $\mathscr{I}_1$. Then for $|\mu|$ small, the series $\sum_{k=1}^{\infty} \mu^k \operatorname{Tr}((-A)^k)/k$ converges and

$$\det(1 + \mu A) = \exp\left[-\sum_{k=1}^{\infty} \mu^k \operatorname{Tr}[(-A)^k]/k\right]$$

Proof Since

$$|\operatorname{Tr}[(-A)^k]| \leq \|A^k\|_1 \leq \|A\|_1 \|A\|^{k-1}$$

the series converges if $|\mu| \|A\|_{\text{op}} < 1$. Moreover, by the product expansion for det and Lidskii's theorem (Theorem XIII.106 and its corollary), we have that, for $|\mu| \max_{1 \leq j \leq N(A)} |\lambda_j(A)| < 1$,

$$\begin{aligned}
\ln[\det(1 + \mu A)] &= \sum_{j=1}^{N(A)} \ln(1 + \mu\lambda_j(A)) \\
&= \sum_{j=1}^{N(A)} \sum_{k=1}^{\infty} (-1)^{k+1} \mu^k \lambda_j(A)^k/k \\
&= \sum_{k=1}^{\infty} (-1)^{k+1} \mu^k \left[\sum_{j=1}^{N(A)} \lambda_j(A)^k\right]/k \\
&= -\sum_{k=1}^{\infty} \mu^k \operatorname{Tr}((-A)^k)/k
\end{aligned}$$

In the above we have used the convergent expansion for $\ln(1 + x)$ on $\{x \mid |x| < 1\}$. The interchanging of the sums is easy to justify by showing that the double sum is absolutely convergent because $\sum |\lambda_j(A)| < \infty$ and $|\mu| \max |\lambda_j(A)| < 1$. ∎

Lemma 7 Let $f(z)$ be analytic for z small with

$$f(z) = \sum_{n=1}^{\infty} (-1)^{n+1} b_n \frac{z^n}{n}$$

Let

$$g(z) \equiv \exp(f(z)) = \sum_{m=0}^{\infty} B_m \frac{z^m}{m!}$$

Then $B_0 = 1$ and B_m is given by the $m \times m$ determinant:

$$B_m = \begin{vmatrix} b_1 & m-1 & 0 & \cdots & 0 \\ b_2 & b_1 & m-2 & \cdots & 0 \\ b_3 & b_2 & b_1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ b_{m-1} & b_{m-2} & b_{m-3} & \cdots & 1 \\ b_m & b_{m-1} & b_{m-2} & \cdots & b_1 \end{vmatrix} \tag{198}$$

Proof Since $g'(z) = f'(z)g(z)$, the power series are related by

$$B_n = \sum_{k=1}^{n} b_k B_{n-k} (-1)^{k+1} \left(\frac{(n-1)!}{(n-k)!} \right) \tag{199}$$

(198) clearly holds for $m = 1$; and if it holds for $B_1, \ldots, B_{m-1}$, then (199) is just the expansion in minors in the first column on the right-hand side of (198). Thus (199) holds by induction. ∎

Theorem XIII.108 (the Plemelj–Smithies formulas) Define $\alpha_m(A)$ and $\beta_m(A)$ by

$$\det(1 + \mu A) = \sum_{m=0}^{\infty} \mu^m \frac{\alpha_m(A)}{m!}$$

$$D_\mu(A) = \sum_{m=0}^{\infty} \mu^m \frac{\beta_m(A)}{m!}$$

Then $\alpha_m(A)$ is given by the $m \times m$ determinant:

$$\alpha_m(A) = \begin{vmatrix} \operatorname{Tr}(A) & m-1 & 0 & \cdots & 0 \\ \operatorname{Tr}(A^2) & \operatorname{Tr}(A) & m-2 & \cdots & 0 \\ \operatorname{Tr}(A^3) & \operatorname{Tr}(A^2) & \operatorname{Tr}(A) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & & 1 \\ \operatorname{Tr}(A^m) & \operatorname{Tr}(A^{m-1}) & \operatorname{Tr}(A^{m-2}) & \cdots & \operatorname{Tr}(A) \end{vmatrix} \tag{200}$$

and $\beta_m(A)$ is given by the $(m+1) \times (m+1)$ determinant

$$\beta_m(A) = \begin{vmatrix} A & m & 0 & \cdots & 0 \\ A^2 & \operatorname{Tr}(A) & m-1 & \cdots & 0 \\ A^3 & \operatorname{Tr}(A^2) & \operatorname{Tr}(A) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A^m & \operatorname{Tr}(A^{m-1}) & \operatorname{Tr}(A^{m-2}) & \cdots & 1 \\ A^{m+1} & \operatorname{Tr}(A^m) & \operatorname{Tr}(A^{m-1}) & \cdots & \operatorname{Tr}(A) \end{vmatrix} \tag{201}$$

where (201) is to be interpreted in the sense that $(\varphi, \beta_m(A)\psi)$ is given by the numerical determinant obtained by replacing A^j by $(\varphi, A^j\psi)$ on the right-hand side of (201).

Proof (200) follows directly from Lemmas 6 and 7. For small μ, we have

$$D_\mu(A) = (A - \mu A^2 + \mu^3 A^2 - \cdots) \det(1 + \mu A)$$

on account of the geometric series expansion of $A(1 + \mu A)^{-1}$. Thus

$$\beta_m(A) = m! \left[A \frac{\alpha_m(A)}{m!} - A^2 \frac{\alpha_{m-1}(A)}{(m-1)!} + \cdots \right]$$

Expanding the right-hand side of (201) in minors in the first column and using (200), we conclude that (201) holds. ∎

As a final abstract result, we use the machinery we have developed thus far to say something about completeness of generalized eigenvectors for a special class of operators in $\mathscr{I}_1$.

Theorem XIII.109 Let A be a trace class operator that is also strictly m-accretive, that is, there is $\varepsilon > 0$ so that

$$\operatorname{Arg}[(\varphi, A\varphi)] \leq \frac{\pi}{2} - \varepsilon$$

for all $\varphi \in \mathscr{H}$. Then the generalized eigenvectors for A span $\mathscr{H}$.

Proof We shall prove that the generalized eigenvectors associated with nonzero eigenvalues span $\overline{\operatorname{Ran} A}$ and then that $\overline{\operatorname{Ran} A} + \operatorname{Ker} A = \mathscr{H}$. Let $\mathscr{M}$ be the span of the generalized eigenvectors associated to nonzero eigenvalues. Since A leaves $\mathscr{M}$ invariant, A^* leaves $\mathscr{M}^\perp$ invariant. Let B be the restriction of A^* to $\mathscr{M}^\perp$. We shall show that $B = 0$, so that $\varphi \in \mathscr{M}^\perp$ implies $A^*\varphi = 0$, which implies that $\varphi \in (\operatorname{Ran} A)^\perp$. So $\mathscr{M}^\perp \subset (\operatorname{Ran} A)^\perp$ and thus $\overline{\operatorname{Ran} A} \subset \mathscr{M}$.

We first claim that $\sigma(B) = \{0\}$. For suppose $\lambda \in \sigma(B)$ with $\lambda \neq 0$. Then, λ is an eigenvalue of B since B is compact as the restriction of the compact operator A^*. Therefore, there is a nonzero $\varphi \in \mathscr{M}^\perp$ with $A^*\varphi = \lambda\varphi$. It follows that $\varphi \in \operatorname{Ran}(A - \bar{\lambda})^\perp$ and that $\bar{\lambda} \in \sigma(A)$. Let P be the spectral projection for $\bar{\lambda}$. Then $\operatorname{Ran} P \subset \mathscr{M}$ so $\varphi \in (\operatorname{Ran} P)^\perp$. But since $\bar{\lambda} \notin \sigma(A \restriction (1-P)\mathscr{H})$, $\operatorname{Ran}(1-P) \subset \operatorname{Ran}(A - \bar{\lambda})$ so $\varphi \in \operatorname{Ran}(1-P)^\perp$. It follows that $\varphi = 0$ since $\operatorname{Ran} P + \operatorname{Ran}(1-P) = \mathscr{H}$. Thus, B can contain only zero in its spectrum.

Let $\varphi \in \mathscr{M}^\perp$. Define the vector-valued analytic function

$$F(\mu) = (1 - \mu B)^{-1}\varphi = -\mu^{-1}(B - \mu^{-1})^{-1}\varphi$$

Since $\sigma(B) = \{0\}$, F is an entire function. Moreover, since B has no nonzero eigenvalues, $\det(1 - \mu B) = 1$ by Theorem XIII.106, and so, by (196),

$$\|F(\mu)\| \leq \exp(|\mu| \, \|B\|_1)\|\varphi\| \tag{202}$$

Since B is m-accretive, we know by Theorem VIII.17 that

$$\|(B - \lambda)^{-1}\| \leq [\operatorname{dist}(\lambda, \{z \mid |\arg z| \leq \tfrac{1}{2}\pi - \varepsilon)]^{-1}$$

Thus, for $|\arg \lambda| \geq \frac{1}{2}\pi - \frac{1}{2}\varepsilon$,

$$\|(B - \lambda)^{-1}\varphi\| \leq |\lambda|^{-1}\csc(\tfrac{1}{2}\varepsilon)\|\varphi\|$$

It follows, that for $|\arg \mu| \geq \frac{1}{2}\pi - \frac{1}{2}\varepsilon$,

$$\|F(\mu)\| \leq \alpha \tag{203}$$

where $\alpha = \|\varphi\|\csc(\frac{1}{2}\varepsilon)$. We claim that (203) holds for all μ. For let $\beta = \frac{1}{2}\pi[\frac{1}{2}\pi - \frac{1}{3}\varepsilon]^{-1}$. For any $C > 0$, the function $F_C(\mu) = F(\mu)\exp(-C\mu^\beta)$ is analytic in the set $D = \{\mu \mid |\arg \mu| \leq \frac{1}{2}\pi - \frac{1}{2}\varepsilon\}$ and goes to zero uniformly as $|\mu| \to \infty$ by (202) and the fact $\beta > 1$ and $\beta(\frac{1}{2}\pi - \frac{1}{2}\varepsilon) < \frac{1}{2}\pi$. Thus, by the maximum modulus principle $|F_C(\mu)|$ takes its maximum values on $\arg \mu = \pm(\frac{1}{2}\pi - \frac{1}{2}\varepsilon)$ where it is bounded by α. Thus, for any $C > 0$ and $\mu \in D$, $|F_C(\mu)| \leq \alpha$, so letting $C \downarrow 0$, we conclude (203). Since (203) holds, $F(\mu)$ is a constant by Liouville's theorem and in particular, $F'(0) = B\varphi$ is zero. Thus $B = 0$, so, by the argument already given, $\overline{\operatorname{Ran} A} \subset \mathscr{M}$.

Now let φ be arbitrary. Let $\psi_n = n^{-1}(A + n^{-1})^{-1}\varphi$ so that $\|\psi_n\| \leq \|\varphi\|$ since A is sectorial. Let ψ be a weak limit point of the ψ_n as $n \to \infty$. We claim that $A\psi = 0$ and $\varphi - \psi_n \in \operatorname{Ran} A$. This will show that $\varphi \in \operatorname{Ker} A + \overline{\operatorname{Ran} A}^{\mathrm{w}}$ where $\overline{}^{\mathrm{w}}$ is the weak closure of $\operatorname{Ran} A$. But, by the Hahn-Banach theorem, $\overline{\operatorname{Ran} A}^{\mathrm{w}} = \overline{\operatorname{Ran} A}$ since $\operatorname{Ran} A$ is a subspace. Thus, the theorem will be proven if we can show $A\psi = 0$ and $\varphi - \psi_n \in \operatorname{Ran} A$.

Fix any η. Then

$$(\eta, A\psi) = \lim_{n\to\infty} \frac{1}{n}\left(\eta, A\left(A + \frac{1}{n}\right)^{-1}\varphi\right)$$

$$= \lim_{n\to\infty} \frac{1}{n}(\eta, \varphi) - \frac{1}{n^2}\left(\eta, \left(A + \frac{1}{n}\right)^{-1}\varphi\right)$$

$$= \lim_{n\to\infty} \frac{1}{n}(\eta, \varphi - \psi_n) = 0$$

since $\|\psi_n\| \leq 1$. This proves that $A\psi = 0$. Furthermore,

$$\varphi - \psi_n = \left[1 - \frac{1}{n}\left(A + \frac{1}{n}\right)^{-1}\right]\varphi = A\left(A + \frac{1}{n}\right)^{-1}\varphi$$

so $\varphi - \psi_n$ is in Ran A. ∎

The methods of this section can sometimes be used to say something about unbounded non-self-adjoint operators.

Corollary Let A be the generator of a holomorphic contraction semigroup and suppose that $(A + 1)^{-1}$ is trace class. Then the generalized eigenvectors for A span $\mathscr{H}$.

Proof By the preceding theorem, it suffices to show that $(A + 1)^{-1}$ is strictly m-accretive since the generalized eigenvectors of A are the same as those of $(A + 1)^{-1}$ (Problem 159). Let $\eta \in \mathscr{H}$ and let $\varphi = (A + 1)^{-1}\eta$. Then

$$(\eta, (A + 1)^{-1}\eta) = ((A + 1)\varphi, \varphi) = \overline{(\varphi, A\varphi)} + (\varphi, \varphi)$$

Thus

$$|\arg(\eta, (A + 1)^{-1}\eta)| \leq \tfrac{1}{2}\pi - \varepsilon$$

if

$$|\arg(\varphi, A\varphi)| \leq \tfrac{1}{2}\pi - \varepsilon$$

Since A is strictly m-accretive, so is $(A + 1)^{-1}$. ∎

The explicit formula for $(1 + \mu A)^{-1}$ when $A \in \mathscr{I}_1$ either in the Plemelj–Smithies form which we have discussed or in the Fredholm form, which we have not discussed, are of limited value because many compact operators of interest are not trace class although they are typically in some $\mathscr{I}_p$ with $p > 1$.

Thus, the extension of the Plemelj–Smithies formula to $\mathscr{I}_p$ is of great interest. The reader is asked to make this extension in Problem 155. The resulting formulas are as simple as those for the trace class case and error estimates are also available. In the examples below we shall sometimes make use of this extended theory.

Example 3 In Section XI.6, we found the scattering amplitude for a potential $V \in R \cap L^1$ in terms of the solution φ of

$$\varphi(x, k) = |V(x)|^{1/2} e^{ikx} - \int K(x, y)\varphi(y, k)\, dy$$

where

$$K(x, y) = (4\pi|x - y|)^{-1} |V(x)|^{1/2} e^{ik|x-y|} V(y)/|V(y)|^{1/2}$$

Notice that since $V \in R$, the operator defined by the kernel K is Hilbert–Schmidt and also that K is *not* self-adjoint. The modified Fredholm theory gives explicit formulas for $\varphi(x, k)$ and $T(k, k')$. These formulas, unlike the Born series (which converges in general only when $|k|$ is large) converge for all $k \notin \mathscr{E}$, the exceptional set.

Example 4 In an example presented at the conclusion of Section VI.5 we showed how to solve the Dirichlet problem for Laplace's equation in $D \subset \mathbb{R}^3$ in terms of the solution of an integral equation with variables in ∂D. There we discussed this equation, viewing it as one on $C(\partial D)$, but one could just as well have considered the equation as one on $L^2(\partial D, dS)$. The kernel in that case is *not* in $\mathscr{I}_1$ or even $\mathscr{I}_2$, but a simple argument shows it is in $\mathscr{I}_4$ and a more subtle argument proves it is in $\mathscr{I}_3$ (or any $\mathscr{I}_{2+\varepsilon}$ with $\varepsilon > 0$) (Problem 160). Thus, one can write down "explicit" solutions for the Dirichlet problem.

Example 5 By Theorem XIII.11, the Schrödinger operator $-d^2/dx^2 + \lambda V$ has a negative eigenvalue for all small positive λ so long as V is nonpositive, in C_0^∞, and not identically zero. The determinants we have introduced in this section turn out to be the natural tool for answering two further questions one might ask about this situation: What if V is not a.e. nonpositive? Is the eigenvalue defined for small λ analytic at $\lambda = 0$? We shall suppose throughout this example that $V \in C_0^\infty$.

By the tool used in Theorem XIII.11, $E < 0$ is an eigenvalue of $p^2 + \lambda V$ if and only if 1 is an eigenvalue of $-\lambda|V|^{1/2}(p^2 - E)^{-1}V^{1/2}$ where

$V^{1/2} = |V|^{1/2}(\text{sgn } V)$. Let $E = -\alpha^2$ for $\alpha > 0$. Then $(p^2 - E)^{-1}$ is an integral operator with integral kernel $(2\alpha)^{-1} \exp(-\alpha|x - y|)$. Define the operators K_α, L_α, M_α with integral kernels:

$$K_\alpha(x, y) = (2\alpha)^{-1}|V(x)|^{1/2} \exp(-\alpha|x - y|)V^{1/2}(y)$$

$$L_\alpha(x, y) = (2\alpha)^{-1}|V(x)|^{1/2}V^{1/2}(y)$$

$$M_\alpha(x, y) = K_\alpha(x, y) - L_\alpha(x, y)$$

Then a simple argument (Problem 161) shows that M_α is trace class not only for $\alpha > 0$ but for all α and is analytic in α. By the argument above, $E < 0$ is an eigenvalue of $p^2 + \lambda V$ if and only if

$$\det(1 + \lambda K_\alpha) = 0 \tag{204}$$

for $\alpha = +\sqrt{|E|}$. Now, the eigenvalue of $p^2 + \lambda V$, if it exists, goes to zero as λ goes to zero since V is a form bounded perturbation of p^2. Since M_α is continuous at $\alpha = 0$, if $\alpha(\lambda)$ is a solution of (204), then $(1 + \lambda M_{\alpha(\lambda)})$ is invertible for all small λ. Thus

$$\det(1 + \lambda K_\alpha) = \det(1 + \lambda M_\alpha) \det(1 + \lambda L_\alpha(1 + \lambda M_\alpha)^{-1})$$

so that (204) is equivalent to

$$\det(1 + \lambda L_\alpha(1 + \lambda M_\alpha)^{-1}) = 0 \tag{205}$$

for λ small. This operator is a rank one operator and for any rank-one operator B, one has (Problem 162)

$$\det(1 + B) = 1 + \text{Tr}(B)$$

Thus (205) is equivalent to

$$F(\alpha, \lambda) \equiv \alpha + \tfrac{1}{2}\lambda(V^{1/2}, (1 + \lambda M_\alpha)^{-1}|V|^{1/2}) = 0 \tag{206}$$

We can now answer the two questions we posed above. F is jointly analytic near $\langle\alpha, \lambda\rangle = \langle 0, 0\rangle$, $(\partial F/\partial\alpha)_{\lambda=0} = 1$, $F(0, 0) = 0$. Therefore, by the implicit function theorem for analytic functions, $F(\alpha, \lambda) = 0$ has a unique solution $\alpha(\lambda)$ for λ near zero with $\alpha(\lambda)$ near 0 and this solution is analytic in λ. We conclude that $p^2 + \lambda V$ has an eigenvalue for all small positive λ if and only if $\alpha(\lambda) > 0$ for λ small and positive. In that case $E(\lambda) = -\alpha(\lambda)^2$ is analytic in λ about $\lambda = 0$. When is $\alpha(\lambda) > 0$? Computing the first two terms in the Taylor series for $\alpha(\lambda)$, we see that

$$\alpha(\lambda) = -\frac{\lambda}{2}\int V(x)\,dx - \frac{\lambda^2}{4}\int V(x)|x - y|V(y)\,dx\,dy + O(\lambda^3)$$

Notice that if the $O(\lambda)$ term in this equation is zero, then the $O(\lambda^2)$ is automatically positive because $-|x-y|$ is conditionally (strictly) positive definite (Problem 163). We summarize:

Theorem XIII.110 Let V be a nonzero function in $C_0^\infty(\mathbb{R})$. Then $-d^2/dx^2 + \lambda V$ has a negative eigenvalue for *all* positive λ if and only if $\int V(x)\,dx \leq 0$, and in that case this eigenvalue is analytic in λ at $\lambda = 0$.

For further discussion of this example including the case where V is neither smooth nor has compact support and the two-dimensional case, where the eigenvalue is *never* analytic at $\lambda = 0$, see the discussion in the Notes and the reference quoted therein.

NOTES

Section XIII.1 The min–max characterization of eigenvalues was first stated as a technical lemma in E. Fischer, "Über Quadratische Formen mit reellen Koeffizienten," *Monatsh. Math. Phys.* **16** (1905), 234–49. H. Weyl in "Das asymptotische Verteilungsgesetz der Eigenwerte linearer partieller Differentialgleichungen," *Math. Ann.* **71** (1911), 441–469, used results very close in spirit to the min–max principle. However, it was R. Courant who in the 1920s first realized the far-reaching consequences of the min–max principle and its power as a tool. The first paper in his series is "Über die Eigenwerte bei den Differentialgleichungen der mathematischen Physik," *Math. Z.* **7** (1920), 1–57.

The extension of the min–max principle from operators with compact resolvent (which was the main application made by Weyl and Courant) to arbitrary operators by using the essential spectrum is something of a folk theorem. Its applications (although not its exact statement) in print go back at least to Kato's *Trans. Amer. Math. Soc.* paper quoted in the Notes to Section 3.

Section XIII.2 Many additional applications of variational methods can be found in S. H. Gould, *Variational Methods for Eigenvalue Problems*, Univ. Toronto Press, Toronto, Canada, 1957, and scattered throughout R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Vols. I, II, Wiley (Interscience), New York, 1953.

The central role of the Rayleigh–Ritz method in the history of variational methods is described by R. Courant in a review talk, "Variational methods for the solution of problems of equilibrium and vibrations," Bull.*Amer. Math. Soc.*, **49** (1943), 1–23:

> Since Gauss and W. Thompson, the equivalence between boundary value problems of partial differential equations on the one hand and problems of the calculus of variations on the other hand has been a central point in analysis. At first, the theoretical interest in existence proofs dominated and only much later were practical applications envisaged by two physicists, Lord Rayleigh and Walter Ritz; they independently conceived the idea of utilizing this equivalence for numerical calculation of the solutions, by substituting for the

variational problems simpler approximating extremum problems in which but a finite number of parameters need to be determined. Rayleigh, in his classic work—*Theory of Sound*—and in other publications, was the first to use such a procedure. But only the spectacular success of Walter Ritz and its tragic circumstances caught the general interest. In two publications in 1908 and 1909, Ritz, conscious of his imminent death from consumption, gave a masterly account of the theory, and at the same time applied his method to the calculation of the nodal lines of vibrating plates, a problem of classical physics that previously had not been satisfactorily treated.

Rayleigh's *Theory of Sound* has been reprinted by Dover, New York, 1945. The two papers by W. Ritz are "Über eine neue Methode zur Lösung gewisser Variationsprobleme der mathematischen Physik.," *J. Reine Angew. Math.* **135** (1908), 1–61, and "Theorie der Transversalschwingungen einer quadratischen Platte mit freien Rändern," *Ann. Physik.* **28** (1909), 737–786. Ritz obtained for his method convergence theorems that are similar in form to Theorem XIII.4.

Temple's inequality first appeared in G. Temple, "The theory of Rayleigh's principle as applied to continuous systems," *Proc. Roy. Soc.* **119A** (1928), 276–293. Temple actually proved several inequalities for a specific problem. The wide applicability and high accuracy of the estimate of Theorem XIII.5 was first emphasized in T. Kato, "On the upper and lower bounds of eigenvalues," *J. Phys. Soc. Japan* **4** (1949), 334–339. The simple proof we give which uses some of Kato's ideas is due to T. Kinoshita in his first paper on the helium atom (see below).

Temple's inequality is a useful tool in perturbation theory. This has been emphasized by E. Harrel, II, Thesis, Princeton Univ., Princeton, New Jersey, 1976. For example, it is easy to prove using Temple's inequality that if E_0, the ground state energy of some operator H_0, is nondegenerate and discrete, and if V is a regular perturbation, then the perturbed eigenvector $\psi_n(\lambda)$ given correctly to order n, gives the perturbed energy $E(\lambda)$ to order $2n + 1$ when placed in the expression $E(\lambda) \simeq (\psi(\lambda), \psi(\lambda))^{-1}(\psi(\lambda), H(\lambda)\psi(\lambda))$ (Problem 12).

There are a wide variety of other lower bound techniques. The pre-1950 situation is summarized by Kato: "the formula given by Temple is the most precise one among them notwithstanding that it was the oldest as well as the simplest one." Three recent techniques of interest in quantum theory are the Bazley technique, the Löwdin technique, and the Thirring technique. Bazley's technique is based on a method developed by Weinstein to compute bounds on frequencies of vibration of clamped plates. This technique first appeared in A. Weinstein, "Étude des spectres des équations aux dérivées partielles de la théorie des plaques élastique," *Mémor. Sci. Math.*, No. 88, 1937. Bazley first applied the method to quantum mechanics in N. Bazley, "Lower bounds for eigenvalues with application to the helium atom," *Phys. Rev.* **120** (1958), 144–149. The method was further developed in papers of Bazley and D. Fox, "Lower bounds for eigenvalues of Schrödinger's equation," *Phys. Rev.* **124** (1961), 483–492; "A procedure for estimating eigenvalues," *J. Mathematical Phys.* **3** (1962), 469–471; and "Lower bounds for energy levels of molecular systems," *J. Mathematical Phys.* **4** (1963), 1147–1153. Löwdin's technique was developed in P.-O. Löwdin, "Studies in perturbation theory X, XI" *Phys. Rev.* **139A** (1965), 357–372; *J. Chem. Phys.* **43S** (1965), 175–185. A comparison of the two methods as applied to an x^4 oscillator is found in C. Reid, "Lower bounds for the energy levels of anharmonic oscillators," *J. Chem. Phys.* **43S** (1965), 180–189 (see especially footnote 4a).

Thirring's bounds are given in W. Thirring, *Vorlesungen über Matematische Physik, T7, Quantenmechanik*, Univ. Wien Lecture Notes, Section 2.9. His bounds include Temple's inequality as a special case and also the following (Problem 13): If ψ is the ground state for H_0 and $V \geq 0$, then

$$H_0 + (\psi, V^{-1}\psi)^{-1}(\psi, \cdot)\psi \leq H_0 + V$$

In particular, if the ground state energy is discrete and nondegenerate, then the ground state energy $E(\lambda)$ of $H_0 + \lambda V$ obeys

$$\lambda(\psi, V^{-1}\psi)^{-1} \leq E(\lambda) - E(0) \leq \lambda(\psi, V\psi)$$

so long as $\lambda(\psi, V^{-1}\psi)^{-1} \leq d$, the distance of $E(0)$ from the rest of the spectrum of H_0.

Except for Thirring's bounds, these methods do not provide very satisfactory bounds for systems with a large number of particles. For atoms, it is possible to use special properties of the Coulomb potential, see P. Hertel, E. Lieb, and W. Thirring, "Lower bound to the energy of complex atoms," *J. Chem. Phys.* **62** (1975), 3355–3356.

For applications of lower bound techniques to membrane and plate problems, see Weinstein's memoir, the recent book, A. Weinstein and W. Stenger, *Methods of Intermediate Problems for Eigenvalues: Theory and Ramifications*, Academic Press, New York, 1971; H. F. Weinberger, "Lower bounds for higher eigenvalues by finite difference methods;" *Pacific J. Math.* **8** (1958), 339–368; and J. Hersch, "Lower bounds for all eigenvalues by cell functions: A refined form of H. F. Weinberger's method," *Arch. Rational Mech. Anal.* **12** (1963), 361–366.

The application of Rayleigh–Ritz methods to the helium atom was first made by G. W. Kellner, "Die Ionisierungsspannung des Heliums nach der Schrödingerschen Theorie," *Z. Phys.* **44** (1927), 91–109. Systematic development of accurate test functions are due to E. Hylleraas in three fundamental papers, "Über den Grundzustand des Helium Atoms," *Z. Phys.* **48** (1928), 469–494; "Neue Berechnung der Energie das Heliums im Grundzustande, sowie des tiefsten Terms von Ortho-Helium," *Z. Phys.* **54** (1929), 347–366; and "Über den Grundterm der Zweielektronenprobleme von H^-, He, Li^+, Be^{++}, usw.," *Z. Phys.* **65** (1930), 209–225. For a delightful personal history of the problem, see E. Hylleraas, "Reminiscences from early quantum mechanics of two-electron atoms," *Rev. Modern Phys.* **35** (1963), 421–436.

A detailed discussion of relativistic corrections to the helium atom together with their history can be found in H. Bethe and E. Salpeter, *Quantum Mechanics of One and Two Electron Atoms*, Springer-Verlag, Berlin and New York, 1957.

With the availability of very accurate experimental data due to work of G. Herzberg, interest revived in the calculation of the ionization energy of helium as a test of QED. The first computations to high accuracy appeared in T. Kinoshita, "Ground state of the helium atom, I, II," *Phys. Rev.* **105** (1957), 1490–1502; **115** (1959), 366–374. More accurate calculations can be found in C. L. Pekeris, "Ground state of two-electron atoms," *Phys. Rev.* **112** (1958), 1649–1658; "1^1S and 2^3S states of helium," *Phys. Rev.* **115** (1959), 1216–1221, and "1^1S, 2^1S and 2^3S states of H^- and He," *Phys. Rev.* **126** (1962), 1470–1476. The last paper can be consulted for experimental and Lamb shift computational references.

Section XIII.3 Theorem XIII.6 (in a slightly weaker form) appears in the book by Courant and Hilbert (Notes to Section 1). Our proof is taken from B. Simon, "On the infinitude or finiteness of the number of bound states for an N-body quantum system," *Helv. Phys. Acta* **43** (1970), 607–630. The example of the three-body system for which $N(\lambda)$ alternates between finite and infinite values is also found in this paper. Additional discussion concerning Theorem XIII.6 can be found in L. Faddeev, "On the expansion of arbitrary functions in eigenfunctions of the Schrödinger operator," *Vestnik Leningrad Univ., Mat. Meh. Astronoma* **7** (1957), 164–172, and in the Birman paper quoted below in connection with the Birman–Schwinger bound.

That the model helium Hamiltonian has an infinite discrete spectrum was proven in T. Kato, "On the existence of solutions of the helium wave equation," *Trans. Amer. Math. Soc.* **70** (1951), 212–218. Zhislin's theorem (Theorem XIII.7) appeared first in G. Zhislin, "Discussion of the spectrum of the Schrödinger operator for systems of many particles," *Trudy Moskov. Mat. Obšč.* **9** (1960), 81–128. Additional discussion of this theorem, extensions to subspaces of fixed

symmetry, and alternative proofs can be found in Simon's paper and in J. Uchiyama, "On the discrete eigenvalues of the many particle systems," *Publ. Res. Inst. Math. Sci.* **A2** (1966/67), 117–132; G. Zhislin and A. Sigalov, "On the spectrum of an energy operator for atoms with fixed nuclei in subspaces corresponding to irreducible representations of permutation groups," *Izv. Akad. Nauk SSSR Ser. Mat.* **29** (1965), 853–860; and E. Balslev, "Spectral theory of Schrödinger operators of many body systems with permutation and rotation symmetries," *Ann. Phys.* **73** (1972), 49–107.

There are a variety of situations where one can prove that a multiparticle system has finitely many eigenvalues in its discrete spectrum including the case of certain negatively charged ions. For example, see J. Uchiyama, "Finiteness of the number of discrete eigenvalues of the Schrödinger operator for a three particle system," *Publ. Res. Inst. Math. Sci.* **A5** (1969), 51–63; G. M. Zhislin, "On the finiteness of the discrete spectrum of the energy operator of negative atomic and molecular ions," *Teoret. Mat. Fiz.* **21** (1971), 332–341 (*Theoret. and Math. Phys.* **7** (1971), 571–578); D. R. Yafaev, "The point spectrum in the quantum-mechanical problem of many particles," *Funkcional. Anal. i Priložeh* **6** (1972), 103–104 (*Functional. Anal. Appl.* **6** (1972), 349–350); M. A. Antonets, G. M. Zhislin, and I. A. Shereshevskii, "On the discrete spectrum of the Hamiltonian of an N-particle quantum system," *Teoret. Mat. Fiz.* **16** (1973), 235–246 (*Theoret and Math. Phys.* **16** (1974), 800–809); I. Sigal, "On the point spectrum of the Schrödinger operators of multiparticle systems," *Commun. Math. Phys.* **48** (1976), 137–154; B. Simon, "Geometric methods in multiparticle quantum systems," CMP (1977); and R. Hill, "Proof that the H^- ion has only one bound state," *Phys. Rev. Lett.* **38** (1977), 643–646.

Theorem XIII.8 is a classical result, although its proof usually rests on a detailed analysis of the behavior of the zeros of $u_\ell(r; E)$ rather than on the min–max principle. The idea of applying Theorem XIII.8 to obtain bounds on $n_\ell(V)$ and the bound in Theorem XIII.9a appears in V. Bargmann, "On the number of bound states in a central field of forces," *Proc. Nat. Acad. Sci. U.S.A.* **38** (1952), 961–966. Bargmann's work was partially motivated by a theorem in R. Jost and A. Pias, "On the scattering of a particle by a static potential," *Phys. Rev.* **82** (1951), 840–850, who proved that $N(V) = 0$ if $\int r|V(r)|\,dr < 1$. Actually, by a general argument (Problem 23), the Jost–Pias result implies Bargmann's bound. Calogero's bound and Theorem XIII.9d first appeared in F. Calogero, "Upper and lower limits for the number of bound states in a given central potential," *Comm. Math. Phys.* **1** (1965), 80–88. For further discussion, see Calogero's book, *Variable Phase Approach to Potential Scattering*, Academic Press, New York, 1967. Theorem XIII.9c is due to V. Glaser, A. Martin, H. Grösse, and W. Thirring, "A family of optimal conditions for the absence of bound states in a potential," in *Studies in Mathematical Physics: Essays in honor of V. Bargmann* (E. Lieb, B. Simon, A. S. Wightman, eds.), Princeton Univ. Press, Princeton, New Jersey, 1976. In the same volume there is a review article by B. Simon, "On the number of bound states of two-body Schrödinger operators: A review." Theorem XIII.9e and a similar bound, $A\lambda^{3/2} < N(\lambda V) < B\lambda^{3/2}$ for large λ, are due to B. Simon, "On the growth of the number of bound states with increase in potential strength," *J. Mathematical Phys.* **10** (1969), 1123–1126. Formulas for the asymptotic behavior of $N(\lambda V)$ are discussed in Section 15. The reader should consult the Notes to Section 15 for references.

The Birman–Schwinger bound was discovered independently by M. Birman, "The spectrum of singular boundary problems," *Math. Sb.* **55** (1961), 124–174 (*Amer. Math. Soc. Trans.* **53** (1966), 23–80), and by J. Schwinger, "On the bound states of a given potential," *Proc. Nat. Acad. Sci. U.S.A.* **47** (1961), 122–129. There have been a variety of refinements of the Birman–Schwinger theorem. For references, consult the review article by Simon quoted above.

The first bounds on $N(V)$ for $n \geq 3$ having the right large coupling behavior were obtained by B. Simon in "Weak trace ideals and the number of bound states of Schrödinger operators," *Trans. Amer. Math. Soc.* **224** (1976), 367–380, who proved that for $n \geq 3$, $N(V) \leq c_{n,\varepsilon}(\|V_-\|_{n/2+\varepsilon} + \|V_-\|_{n/2-\varepsilon})^{n/2}$ for a constant $c_{n,\varepsilon}$ diverging as $\varepsilon \to 0$. Here $\|\ \|_p$ is the $L^p(\mathbb{R}^n)$

norm. Independently and by a different method, A. Martin, in "A Bound on the total number of bound states in a potential," proved that $N(V) \leq (2\pi)^{-1}(\|V_-\|_1\|V_-\|_2^2)^{1/3}$ in three dimensions. The Cwikel–Lieb–Rosenbljum bounds which imply the Simon and Martin bounds (except for the possible size of constants) appear independently in M. Cwikel, "Weak type estimates for singular values and the number of bound states of Schrödinger operators," *Ann. Math.* **106** (1977), 93–100. E. Lieb, "The number of bound states of one-body Schrodinger operators and the Weyl problem." (to appear), and G. V. Rozenbljum, "The distribution of the discrete spectrum for singular differential operators," *Dokl. Akad. Nauk SSSR* **202** (1972), 1012–1015.

Lieb also provides new proofs of bounds on the sum of powers of the negative eigenvalues of $-\Delta + V$. Such bounds had been proven earlier by E. Lieb and W. Thirring; see Problems 31–33. The Cwikel–Lieb–Rosenbljum and Lieb–Thirring bounds are especially interesting on account of the phase-space intuition discussed in Section 15.

The proof we give of the Cwikel–Lieb–Rosenbljum bound is a simple variant of Lieb's due to him (unpublished). Cwikel's proof was based on Theorem XI.22.

The bounds of Lieb and Thirring on the sum of the negative eigenvalues of $-\Delta + V$, which are proven using the Birman–Schwinger bound on $N_E(V)$, are especially interesting because they are an important part of a simple proof of the "stability of matter"; see E. Lieb and W. Thirring, "Bound for the kinetic energy of fermions which proves the stability of matter." *Phys. Rev. Lett.* **35** (1975), 687–689.

Section XIII.4 H. Weyl in "Über beschränkte quadratische Formen, deren Differenz vollstetig ist," *Rend. Circ. Mat. Palermo* **27** (1909), 373–392, proved (what would be in modern terminology) Theorem XIII.14 in case A and B are bounded self-adjoint operators with $A - B$ compact. For non-self-adjoint operators, there are many distinct definitions of essential spectrum and a variety of forms of Weyl's theorem. For example on pp. 242–244 of Kato's *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin and New York, 1966, there is a discussion of a notion of $\sigma_{ess}(A)$ so that $\sigma_{ess}(A) = \sigma_{ess}(B)$ whenever $A - B$ is compact. If B is the operator in Example 1, according to Kato's definition $\sigma_{ess}(B)$ is the unit circle $\{z \mid |z| = 1\}$ while according to our definition, $\sigma_{ess}(B)$ is the unit disk $\{z \mid |z| \leq 1\}$. For an introduction to the literature on various kinds of essential spectra, see K. Gustafson, "Necessary and sufficient conditions for Weyl's theorem," *Michigan Math. J.* **19** (1972), 71–81.

The meromorphic Fredholm theorem in its full generality appeared in M. Ribaric and I. Vidav, "Analytic properties of the inverse $A(z)^{-1}$ of an analytic linear operator-valued function $A(z)$," *Arch. Rational Mech. Anal.* **32** (1969), 298–310. In this paper, the theorem is proven for operators on an arbitrary Banach space.

Corollary 3 to Theorem XIII.14 is a combination of results of M. Schechter, "On the essential spectrum of an arbitrary operator, I," *J. Math. Anal. Appl.* **13** (1966), 205–215, who proved the case $n = 2$ and K. Gustalfson and J. Weidmann, "On the essential spectrum," *J. Math. Anal. Appl.* **25** (1969), 121–127. An alternate "direct" proof can be found in J. Weidmann, "Spectral theory of partial differential operators," in *Spectral Theory and Differential Equations*, (W. N. Everitt, ed.), Lecture Notes in Mathematics, No. 448, Springer-Verlag, Berlin and New York, 1974.

Results related to Corollary 4 of Theorem XIII.14 and extensions of the ideas including A's that are not bounded below can be found in G. Nenciu, "Self-adjointness and invariance of the essential spectrum for Dirac operators defined as quadratic forms," *Comm. Math. Phys.* **48** (1976), 235–247.

For additional discussion of the essential spectrum of one-body Schrödinger operators see Problem 41; E. Balslev, "The singular spectrum of elliptic differential operators in $L^p(\mathbb{R}^n)$," *Math. Scand.* **19** (1966), 193–210; P. Rejto, "On the essential spectrum of the hydrogen energy

and related operators," *Pacific J. Math.* **19** (1966), 109–140 and M. Schechter, *Spectra of Partial Differential Operators*, North Holland, Amsterdam, 1972.

The ideas in Example 8 are taken from J. E. Avron and I. W. Herbst, "Spectral and scattering theory of Schrödinger operators related to the Stark effect," *Comm. Math. Phys.* **52** (1977), 239–254. In the one-dimensional case, where the theory of ordinary differential equations can be exploited, one can prove that $\sigma(-d^2/dx^2 + W) = (-\infty, \infty)$ for a more general class of potentials W than those of the form $x + V$ with V short range. See, for example, E. C. Titchmarsh, *Eigenfunctions Expansions Associated with 2nd Order Differential Equations*, Oxford Univ. Press (Clarendon), London and New York, 1948; K. Kodaira, "The eigenvalue problem for ordinary differential equations of second order and Heisenberg's theory of *S*-matrices", *Amer. J. Math.* **71** (1949), 921–945; J. Weidmann, "Zur Spektraltheorie von Sturm–Liouville Operatoren," *Math. Z.* **98** (1967), 286–302; M. A. Neumark, *Lineare Differentialoperatoren*, Akad-Verlag, Berlin, 1960; J. Walter, "Absolute continuity of the essential spectrum of $-d^2/dx^2 + q(x)$ without monotony of q," *Math. Z.* **129** (1972), 83–94; P. Rejto, "On a theorem of Titchmarsh–Neumark–Walter concerning absolutely continuous operators, I, II," *Lett. Mat. Phys.* **1** (1975), 49–56, 57–66.

Section XIII.5 The HVZ theorem is named for W. Hunziker, C. Van Winter, and G. Zhislin for their work in the fundamental papers: W. Hunziker, "On the spectra of Schrödinger multiparticle Hamiltonians," *Helv. Phys. Acta* **39** (1966), 451–462; C. Van Winter, "Theory of finite systems of particles, I," *Mat.-Fys. Skr. Danske Vid. Selsk* **1** (8) (1964), 1–60; and G. Zhislin, "Discussion of the spectrum of the Schrödinger operator for systems of many particles," *Tr. Mosk. Mat. Obs.* **9** (1960), 81–128. Zhislin proved the result that $\sigma_{ess} = [\Sigma, \infty)$ for a restricted class of systems that included atomic Hamiltonians. His method has been further discussed by K. Jörgens, "Zur Spektraltheorie der Schrödinger Operatoren," *Math. Z.* **96** (1967), 355–372 and K. Jörgens and J. Weidmann, *Spectral Properties of Hamiltonian Operators*, Lecture Notes in Mathematics, No. 319, Springer-Verlag, Berlin and New York, 1973. Van Winter developed the Weinberg–Van Winter equations and (implicitly) proved the HVZ theorem in case $V \in L^2$ by employing the theory of integral equations with Hilbert–Schmidt kernels. Hunziker proved the $L^2 + (L^\infty)_\epsilon$ case in work which was independent of Van Winter. The Rollnik potential case first appeared in B. Simon, *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms*, Princeton Univ. Press, Princeton, New Jersey, 1972.

The Weinberg–Van Winter equations (in the form (24) rather than in the form (29)) and a generalization to N-body systems appeared in the paper of Van Winter quoted above and, independently in S. Weinberg, "Systematic solution of multiparticle scattering problems," *Phys. Rev.* **133** (1964), 232–256. Weinberg proved compactness of $I(E)$ only for three-body systems. The compactness for arbitrary N appears in Van Winter (when $V \in L^2$) and, independently, in W. Hunziker, "Proof of a conjecture of S. Weinberg," *Phys. Rev.* **135B** (1964), 800–803. Our proof of this fact (Lemma 4B) and in particular, the use of Lemma 5 are taken from Simon's monograph (see above). The symmetrized versions of the equations (29) which are needed if $V_{ij} \in R \backslash L^2$, also come from Simon's monograph.

Another set of equations for the resolvent, also with compact kernel are the Faddeev–Yakubovsky equations which appear for $N = 3$ in L. Faddeev, "Mathematical questions in the quantum theory of scattering for three particle systems," *Trudy Mat. Inst. Steklov* **69** (1963) [transl. Israel Program for Scientific Translation, 1965] and for arbitrary N in O. A. Yakubovsky, "On the integral equations in the theory of N-particle scattering," *Soviet J. Nuclear Phys.* **5** (1967), 937–942. The F-Y equations are much more complicated than the W-V equations, but they cannot have "spurious zeros" of the type discussed below. This makes them more useful in scattering theory. Still another set of equations (also without spurious zeros)

appears in R. G. Newton, "Equations with connected kernels for N-particle T-operators," *J. Mathematical Phys.* **8** (1967), 851–856.

In the proof of the HVZ theorem, we saw that $\sigma_{\text{disc}}(H) \subset \{z \mid 1 - I_R(z) \text{ is not invertible}\}$. In fact, if $H\psi = E\psi$, then $I_R(E)[(H_0 - E)^{1/2}\psi] = (H_0 - E)^{1/2}\psi$. However, it can happen that $1 - I_R(E)$ is not invertible for some $E \in \rho(H)$. This was first pointed out in P. Federbush, "Existence of spurious solutions to many body Bethe–Salpeter equations," *Phys. Rev.* **148** (1966), 1551–1552, and is further discussed in R. Newton, "Spurious solutions of three particle equations," *Phys. Rev.* **153** (1967), 1502. Such values of E are called "spurious zeros." The reason for the name is that for $(1 - I_R(E))^{-1}$ to have a pole without $R(E) = (1 - I_R(E))^{-1}D_R(E)$ having a pole, $D_R(E)$ and $1 - I_R(E)$ must have compensating "zeros." Thus "zeros" of $1 - I_R(E)$ (or more precisely, of the Fredholm determinant $\det(1 - I_R(E))$) may occur at noneigenvalues.

The second proof we give of Theorem XIII.17 is a descendant of the original proof of Zhislin and a variant of a proof of V. Enss, "A Note on Hunziker's Theorem," *Comm. Math. Phys.* **52** (1977), 233–238. We closely follow the presentation of B. Simon, "Geometric methods in multiparticle quantum systems," in press. One technical simplification over the development of Zhislin, Jörgens and Weidmann, and Enss is the use of Theorem XIII.77 (Lemma 7 in this section) in place of a Weyl criterion.

Theorems of the genre of Theorem XIII.17′, dealing with the HVZ theorem when one restricts to symmetry subspaces, have been discussed in the articles of Zhislin and Sigalov, Balslev, and Simon quoted in the Notes to Section 3, in the monograph of Jörgens and Weidmann quoted above, and in the paper of Simon just quoted.

Section XIII.6 Our discussion of what we call the Aronszajn–Donoghue theory closely follows that in W. F. Donoghue, "On the perturbation of spectra," *Comm. Pure Appl. Math.* **18** (1965), 559–579, who remarks that his results are essentially contained in N. Aronszajn, "On a problem of Weyl," *Amer. J. Math.* **79** (1957), 597–610. D. Pearson has found $V \in C^\infty$, $D^jV \to 0$ at $\pm\infty$ so that $-D^2 + V$ has purely singular continuous spectrum.

Section XIII.7 The theory of smooth operators was developed by T. Kato in two remarkable papers, "Wave operators and similarity for some non-self-adjoint operators," *Math. Ann.* **162** (1966), 258–279, and "Smooth operators and commutators," *Studia Math.* **31** (1968), 535–546. In the first paper Kato defined "H-smooth" and proved Theorems XIII.22 (in a stronger form; see Problem 49), XIII.23 (implicitly), XIII.24, XIII.25, XIII.26 (in a stronger form; see Problems 53, 54 and the discussion below), and XIII.27 (in the case $N = 2$). The second paper contains a criterion for H-smoothness if H is bounded—in case H is multiplicity free, this is the criterion of Example 4 and Problem 50—and Kato's proof of the Putnam–Kato theorem (Theorem XIII.28). Our proofs of these results are patterned on Kato's arguments.

What we call Kato's smoothness theorem appears in a stronger form in his *Math. Ann.* paper. First, he proves that $H_0 + \lambda V$ and H_0 are similar, i.e., $W(H_0 + \lambda V)W^{-1} = H_0$ for an invertible bounded operator W even when λ is complex. His proof is based on a "time-independent" formulation of scattering. Second, neither H_0 or V need be self-adjoint. What is important is that $\sigma(H_0) \subset \mathbb{R}$ and $|V|^{1/2}$ be H_0-smooth and H_0^*-smooth in the sense of the basic definition (rather than the equivalent formulations in Theorem XIII.25) and that $\sup_{\mu \notin \mathbb{R}} \| |V|^{1/2}(H_0 - \mu)^{-1}|V|^{1/2}\| < \infty$.

Weak coupling results proving that $-\Delta$ and $-\Delta + V$ are unitarily equivalent for a suitable class of small V first appeared in J. Schwartz, "Some non-self adjoint operators," *Comm. Pure Appl. Math.* **13** (1960), 609–639. Schwartz dealt with the (reduced) two-body case in $\mathbb{R}^m$ with $m \geq 3$ and proved that if $\int (1 + x^2)|D^\alpha V|\, dx < \infty$ for all $\alpha \leq m - 1$, then $-\Delta$ and $-\Delta + \lambda V$ are unitarily equivalent for λ small.

Using the Dyson series (see Section X.12), R. Prosser proved a weak coupling theorem in the two-body case in "Convergent perturbation expansions for certain wave operators," *J. Mathematical Phys.* **5** (1964), 708–713. Kato proved Theorem XIII.27 in the case $N = 2$ in his *Math. Ann.* paper; in particular, (43) was used by Kato. The Prosser and Kato proofs are based on using the series

$$\Omega^- = 1 + i\int_0^\infty V_{s_1}\, ds_1 + i^2 \int_0^\infty \int_0^{s_1} V_{s_2} V_{s_1}\, ds_2\, ds_1 + \cdots$$

where

$$V_s = e^{iH_0 s} V e^{-iH_0 s}$$

for $\Omega^- \varphi$, and the norm estimate

$$\|V_{s_1} V_{s_2} \cdots V_{s_n} \varphi\| = \| |V|^{1/2} \| \, \| |V|^{1/2} e^{i(s_2 - s_1)H_0} |V|^{1/2} \| \cdots \| |V|^{1/2} e^{-is_n H_0} \varphi \|$$

Small coupling results for three-body problems were proven by Hunziker in his Boulder Lectures (see the Notes to Section XI.5) who used Prosser's techniques. He remarked that the techniques could not work for N-body systems with $N \geq 4$ because $\| \, |V_{ij}|^{1/2} e^{isH_0} |V_{k\ell}|^{1/2} \|$ is constant if i, j, k, ℓ are all distinct. The idea of controlling $\int |V_{ij}|^{1/2} e^{isH_0} |V_{k\ell}|^{1/2}\, ds$ which appears under "Case (3)" in our proof of Theorem XIII.27 and thereby the N-body results if $N \geq 4$ is due to R. Iorio and M. O'Carroll, "Asymptotic completeness for multi-particle Schrödinger Hamiltonians with weak potentials," *Comm. Math. Phys.* **27** (1972), 137–145. It is an open conjecture that the conclusion of Theorem XIII.27 holds if $V_{ij} \in L^{m/2}$.

The theorem that H has purely absolutely continuous spectrum if there exists an A with $i[H, A] \geq 0$ appeared first in C. R. Putnam, *Commutation Properties of Hilbert Space Operators and Related Topics*, Springer-Verlag, Berlin and New York, 1967. The proof we give is from Kato's *Studia* paper.

Application of the Kato–Putnam theory to repulsive potentials appeared first in R. Lavine, "Absolute continuity of Hamiltonian operators with repulsive potentials," *Proc. Amer. Math. Soc.* **22** (1969), 55–60. The theory was much further developed (and in particular Theorems XIII.29 and XIII.32 appear) in R. Lavine, "Commutators and scattering theory, I. Repulsive interactions," *Comm. Math. Phys.* **20** (1971), 301–323. Theorem XIII.29 appears in a slightly weaker form (an extra condition that $r\, \partial V/\partial r \ll H_0$ is added). For potentials, repulsive, central, and only $O(r^{-1-\epsilon})$, Lavine has proven the analogue of Theorem XIII.32 in "Completeness of the wave operators in the repulsive N-body problem," *J. Mathematical Phys.* **14** (1973), 376–379. Additional discussion of the two-body repulsive case can be found in M. Arai, "Absolute continuity of Hamiltonian operators with repulsive potentials," *Publ. Res. Inst. Math. Sci.* **7** (1971/72), 621–635. Our proof that $i[A, H_0] \geq 0$ follows Arai's paper.

Theorem XIII.31 and the notion of "H-smooth on Ω" are taken from R. Lavine, "Commutators and scattering theory, II. A class of one-body problems," *Indiana Univ. Math. J.* **21** (1972), 643–656.

The theory of smooth perturbations has been applied to the existence of propagators and scattering theory by E. B. Davies, "Time dependent scattering theory," *Math. Ann.* **210** (1974), 149–162, and extended to a Banach space setting in D. E. Evans, "Smooth perturbations in non-reflexive Banach spaces," *Math. Ann.* **221** (1976), 183–194.

Section XIII.8 Theorem XIII.33 is due to S. Agmon. He announced his results in "Spectral properties of Schrödinger operators," *Proc. Int. Cong. Math. of 1970*, Vol. 2, pp. 679–684, Gauthier-Villars, Paris, 1971. The details appear in S. Agmon, "Spectral properties of Schrödinger operators and scattering theory," *Ann. Scuola Norm. Sup. Pisa Cl. Sci.* **II**, 2 (1975), 151–218.

Our approach is based on a series of lectures by Agmon together with helpful remarks by H. Epstein, J. Ginibre, and R. Lavine. Theorem XIII.33d was proven prior to Agmon in T. Kato and S. Kuroda, "Theory of simple scattering and eigenfunctions expansions" in *Functional Analysis and Related Fields*, Springer-Verlag, Berlin and New York, 1970, 99–131. That (d) follows from Agmon's a priori estimates and the theory of local smoothness is a remark of R. Lavine in the paper quoted below.

Agmon's work represents the culmination of several lines of development. The first involves proving that $\sigma_{sing}(-\Delta + V) = \varnothing$ when V is $O(|x|^{-\mu})$ at ∞ (some of the papers quoted below require additional smoothness conditions). The earliest result was for $\mu > 2$ in the paper of Ikebe quoted in the Notes to Section XI.6. This was successively improved to $\mu > \frac{3}{2}$ by W. Jäger, "Zur Theorie der Schwingungsgleichung mit variablen Koeffizienten in Aussengebieten," *Math. Z.* **102** (1967), 62–88, to $\mu > \frac{4}{3}$ in P. Rejto, "On partly gentle perturbations, III" *J. Math. Anal. Appl.* **27** (1969), 21–67, to $\mu > \frac{5}{4}$ in T. Kato, "Some results on potential scattering," *Proc. Int. Conf. on Functional Analysis and Related Topics*, Tokyo, 1969, 206–215, and to $\mu > \frac{6}{5}$ by P. Rejto in "Some potential perturbations of the Laplacian," *Helv. Phys. Acta* **44** (1971), 708–736, and by S. Kuroda (quoted below). Rejto and Kuroda both modified their methods in response to Agmon's bootstrap argument and were able to handle all $\mu > 1$. Shortly after Agmon, and independently, the case $\mu > 1$ was handled by Y. Saito, "The principle of limiting absorption for second-order differential equations with operator-valued coefficients," *Pub. Res. Inst. Math. Sci.* **7** (1972), 581–619.

A second line of development involved the idea of proving $\sigma_{sing} = \varnothing$ by a perturbation theory of maps from X to X^* where X is a Banach space imbedded in $\mathscr{H}$. We discuss such an idea in the appendix to Section XI.6. This idea was developed by J. S. Howland, "Banach space techniques in the perturbation theory of self-adjoint operators with continuous spectra," *J. Math. Anal. Appl.* **20** (1967), 22–47, and "A perturbation-theoretic approach to eigenfunction expansions," *J. Functional Analysis* **2** (1968), 1–23, and by P. A. Rejto, "On partly gentle perturbations, I–III," *J. Math. Anal. Appl.* **17** (1967), 435–462; **20** (1967), 145–187; **27** (1969), 21–67. The use of weighted L^2 spaces was first advocated (in a slightly different context) by S. Kuroda, "On the Hölder continuity of an integral involving Bessel functions," *Quart. J. Math. Oxford Ser.* **21** (1970), 71–81.

A third line of development involved the abstract theory of eigenfunction expansions of Kuroda (see the Notes to Section XI.6) and the theory of higher order elliptic operators. In fact, Agmon's theory works for a large class of operators (see Problem 70 and below). A theory with similar results was developed (partly independently of Agmon) by S. Kuroda in "Scattering theory for differential operators, I, II," *J. Math. Soc. Japan* **25** (1973), 75–104; 222–234. Let $H_0 = \sum_{|\alpha| \le 2m} a_\alpha (-iD)^\alpha$ where a_α is real. Suppose moreover that H_0 is **elliptic**, that is, $\sum_{|\alpha| = 2m} a_\alpha k^\alpha \neq 0$ for all $k \in \mathbb{R}^n$, $k \neq 0$. Let $P_1(k) = \sum_{|\alpha| \le 2m} a_\alpha k^\alpha$. A point k where grad $P_1 = 0$ is called a critical point and the value of P_1 at such a point is called a **critical value**. It can be shown that H_0 has only finitely many critical values λ_i. Let $V = \sum_{|\alpha| \le 2m} V_\alpha(x)(-iD)^\alpha$ be such that: (i) $|V_\alpha(x)| \le C_\alpha(1 + |x|^2)^{-1/2-\varepsilon}$. (ii) V is formally self-adjoint, i.e., $(\varphi, V\varphi)$ is real for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$. (iii) For each $x \in \mathbb{R}^n$ and $k \in \mathbb{R}^n \backslash \{0\}$, $\sum_{|\alpha| = 2m} (a_\alpha + V_\alpha(x))k^\alpha \neq 0$. Then Agmon and Kuroda have proven the following generalization of Theorem XIII.33:

(a) The eigenvalues of $H_0 + V$ at noncritical values of H_0 are of finite multiplicity and can have only critical values of H_0 as limit points.

(b) If $[a, b]$ is disjoint from all critical values of H_0 and all eigenvalues of $H \equiv H_0 + V$ and if $\delta > \frac{1}{2}$, then

$$\sup_{a \le x \le b;\, 0 < y < 1} \|(H - x - iy)^{-1}\|_{\delta, -\delta} < \infty$$

(c) $\sigma_{sing}(H_0 + V) = \varnothing$.
(d) Wave operators exist and are complete.

Extensions of the Agmon–Kuroda work to a slightly larger class of potentials can be found in S. Agmon and L. Hormander, "Asymptotic properties of solutions of differential equations with simple characteristics," *J. Anal. Math.* **30** (1976), 1–38. These authors use slightly different spaces which they consider more natural.

In Agmon's original work, he does not prove or use the existence of limiting boundary values for $(H_0 - \lambda)^{-1}$ or $(H - \lambda)^{-1}$. Lemmas 6 and 7 were replaced by a limiting argument known as the "principle of limiting absorbtion." The quadratic estimates of Lemma 6 are due to Lavine.

Theorem XIII.33 is capable of generalization in two other directions. First, V need only be form compact (see Problem 71). Secondly, one can discuss the case $V = V_1 + V_2$ where $\partial V_1/\partial r$ and V_2 are $O(r^{1-\varepsilon})$ at ∞. This is done by R. Lavine, "Absolute continuity of positive spectrum for Schrödinger operators with long range potentials," *J. Functional Analysis* **12** (1973), 30–54. See also T. Ikebe and Y. Saito, "The limiting absorbtion method and absolute continuity for the Schrödinger operator," *J. Math. Kyoto* **12** (1972), 513–542, and Y. Saito, "The principle of limiting absorbtion for the non-self-adjoint Schrödinger operator in $\mathbb{R}^n (N \neq 2)$" *Publ. Res. Inst. Math. Sci.* **9** (1974), 397–428.

Further developments of the Agmon–Kuroda theory appear in a series of papers by M. Schechter, "A unified approach to scattering," *J. Math. Pures Appl.* **53** (1974), 373–396; "Scattering theory for elliptic operators of arbitrary order," *Comm. Math. Helv.* **49** (1974), 84–113; "Scattering theory for second order elliptic operators," *Ann. Mat. Pura et Appl.* **55** (1975), 313–331, "Scattering Theory for Elliptic Systems," *J. Math. Soc. Japan* **28** (1976), 71–79; and "Nonhomogeneous elliptic systems and scattering," *Tohoku Math. J.* **27** (1975), 601–616.

The Agmon method has been extended to study $-\Delta + V + \mathbf{a} \cdot \mathbf{x}$ in I. W. Herbst, "Unitary equivalence of Stark Hamiltonians," *Math. Z.* **155** (1977), 55–71. Herbst proves that if $V = V_1 + V_2$ where $V_2 \in L^2(\mathbb{R}^3)$ has compact support, V_1 satisfies $|V_1(x)| \leq C(1 + (\mathbf{a} \cdot \mathbf{x})^2)^{-1/4-\varepsilon}$, and $-\Delta + V + \mathbf{a} \cdot \mathbf{x}$ has no eigenvalues, then $\Omega^{\pm}(-\Delta + V + \mathbf{a} \cdot \mathbf{x}, -\Delta + \mathbf{a} \cdot \mathbf{x})$ exist and are unitary. Avron and Herbst, in their paper quoted in the notes to Section 4, give criteria under which $-\Delta + V + \mathbf{a} \cdot \mathbf{x}$ has no eigenvalues.

Section XIII.9 The theory of commutative Banach algebras is discussed in Chapter XV. The elementary material used in this section may also be found in I. Gel'fand, D. Raïkov, G. Shilov, *Commutative Normed Rings*, Chelsea, New York, 1964, or W. Rudin, *Functional Analysis*, McGraw-Hill, New York, 1973, or many other texts.

Theorem XIII.34 was proven by A. Brown and C. Pearcy in "Spectra of tensor products of operators," *Proc. Amer. Math. Soc.* **17** (1966), 162–166. M. Schechter generalized the Brown–Pearcy result in "On the spectra of operators on tensor products," *J. Functional Analysis* **4** (1969), 95–99, by proving that

$$\sigma(P(A \otimes I, I \otimes B)) = P(\sigma(A), \sigma(B))$$

where A and B are bounded operators and P is a polynomial in two variables. In particular, Schechter introduced the use of double commutant algebras. Subsequently, this spectral mapping theorem was extended to the class of rational functions in two variables analytic in a neighborhood of $\sigma(A) \times \sigma(B)$ in A. Dash and M. Schechter, "Tensor products and joint spectra," *Israel J. Math.* **8** (1970), 191–193.

Ichinose's lemma and generalizations appeared in T. Ichinose "On the spectra of tensor products of linear operators on Banach spaces," *J. Reine Angew. Math.* **244** (1970), 119–153, and "Operators on tensor products of Banach spaces," *Trans. Amer. Math. Soc.* **170** (1972),

197–219; see also "Operational calculus for tensor products of linear operators on Banach spaces," *Hokkaido Math. J.* **4** (1975), 306–334. M. Reed and B. Simon proved a spectral mapping theorem for a large class of unbounded functions of the unbounded operators $A \otimes I$, $I \otimes B$ in "Tensor products of closed operators on Banach spaces," *J. Functional Analysis.* **13** (1973), 107–124. Theorem XIII.35 is a special case of the Ichinose work and the Reed–Simon work. The proof given in Section 9 is new and much simpler than the proof in the Ichinose and Reed–Simon papers; but since it uses the special property that $e^{-t(A+B)} = e^{-tA} \otimes e^{-tB}$, it cannot be used to prove a spectral mapping theorem for more general functions of A and B.

Section XIII.10 There is a connection between the theory of dilation analytic potentials and the methods used in Section XI.8 to discuss analyticity of the partial wave amplitude for generalized Yukawa potentials. This later set of ideas was discussed in an N-body setting by C. Lovelace, "Three particle systems and unstable particles" in *Strong Interactions and High Energy Physics* (R. C. Moorehouse, ed.) Oliver and Boyd, London, 1964, several years before the development of dilation analytic techniques; but the connection between the two approaches was appreciated only later.

The idea of using dilations and the perturbation theory of discrete spectrum to control the singular continuous spectrum was first used by J. M. Combes in an unpublished manuscript, "An algebraic approach to quantum scattering." The idea was developed in the two-body case by J. Aguilar and J. M. Combes, "A class of analytic perturbations for one-body Schrödinger Hamiltonians," *Comm. Math. Phys.* **22** (1971), 269–279, and in the N-body case by E. Balslev and J. M. Combes, "Spectral properties of many-body Schrödinger operators with dilatation analytic interactions," *Comm. Math. Phys.* **22** (1971), 280–294. Both these papers discussed the class C_α (see Problem 73) rather than $\mathscr{F}_\alpha$ but otherwise Theorems XIII.36 and XIII.37 appear in the first and second papers (respectively).

Several years later, unaware of the Balslev–Combes work, C. Van Winter proved similar theorems by a related method in "Complex dynamical variables for multiparticle systems with analytic interactions, I, II," *J. Math. Anal. Appl.* **47** (1974), 633–670; **48** (1974), 368–399. The special role of the dilation group is not apparent in Van Winter's work, which is based on certain spaces of analytic functions.

Because Ichinose stated his theorem in terms of a bound on the resolvents of operators rather than in terms of sectorial operators or holomorphic semigroups, Balslev and Combes proved a bound on the N-body resolvents by a difficult inductive proof rather than by directly appealing to sectoriality. The class $\mathscr{F}_\alpha$ was introduced in B. Simon, "Quadratic form techniques and the Balslev–Combes theorem," *Comm. Math. Phys.* **27** (1972), 1–9. This paper also pointed out that sectorial operator methods allowed simplifications in the proofs and it removed a restriction $|\operatorname{Im} \theta| < \pi/2$ which Balslev and Combes imposed because of their direct reliance on Ichinose's lemma in its original form.

Dilation analytic techniques and, more generally, the technique of continuation in a group parameter play a role in many facets of N-body Hamiltonians and not just in eliminating the continuous singular spectrum. In particular they are of importance in the theory of resonances (Section XII.6), in exponential falloff of eigenfunctions (Section 11), and in eliminating positive eigenvalues (Section 13).

Section XIII.11 Hölder continuity of vectors in $C^\infty(H)$ for suitable N-body Hamiltonians was first proven by T. Kato in "On the eigenfunctions of many-particle systems in quantum mechanics," *Comm. Pure Appl. Math.* **10** (1957), 151–171. Kato's conditions on his potentials are slightly different from $M_\sigma^{(3)}$; namely, he supposes that $V = V_1 + V_2$ where $V_2 \in L^\infty$ and $V_1 \in L^\sigma$ with supp V_1 compact. Kato's proof is in x space and is more complex than the

proof of Theorem XIII.38, but it contains the basic idea of an L^p bootstrap argument. The idea of using p-space techniques is due to B. Simon, "Pointwise bounds on eigenfunctions and wave packets in N-body quantum systems, I," *Proc. Amer. Math. Soc.* **42** (1974), 395–401.

In the paper quoted above, Kato also proves a sharper result on the singularities of atomic wave functions ψ than is given by Theorem XIII.38. Theorem XIII.38 implies only that ψ is uniformly Hölder continuous of order θ for any $\theta < 1$. Kato shows that $\sup_{x \notin C} |\text{grad } \psi(x)| < \infty$ where C is the set of points where some coordinate difference goes to 0, and, in particular, ψ is Lipschitz continuous. Moreover, the discontinuities of grad ψ at coincident points are explicitly computed in terms of the values of ψ at such points.

The sharp results of Theorems XIII.39–XIII.42 are taken from a set of papers that appeared in preprint form in the fall of 1972. Theorems XIII.39 and XIII.40 appeared in A. O'Connor, "Exponential decay of bound state wave functions," *Commun. Math. Phys.* **32** (1973), 319–340. O'Connor's proof is based on Paley–Wiener ideas and the use of the Weinberg–Van Winter equations: It is conceptually simple but kinematically somewhat complex. The proof we give is patterned after that of J. Combes and L. Thomas, "Asymptotic behavior of eigenfunctions for multiparticle Schrödinger operators," *Commun. Math. Phys.* **34** (1973), 251–270. Combes and Thomas, who were motivated by O'Connor's work, noted the applicability of the ideas to nonthreshold eigenvalues of dilation analytic systems. Their results are stated in terms of the group generated by dilations and p-space translations.

Theorem XIII.42 appeared in the paper of Simon quoted at the start of the Notes of this section. Slightly earlier, R. Ahlrichs, "Asymptotic behavior of atomic bound state wave functions," *J. Mathematical Phys.* **14** (1973), 1860–1863, noted that uniform Hölder continuity and L^2 exponential falloff implied pointwise exponential falloff, but perhaps at a slower rate. Simon's work was motivated by the work of Ahlrichs and O'Connor.

Theorem XIII.41 has a sharp form analogous to Theorem XIII.40. For example, one can prove the following (see the Combes–Thomas paper): If each $V_{ij} \in \mathscr{F}_\alpha$ with $\alpha > \pi/4$ and if $\sum (i\pi/4)$ is the set of thresholds for $H(i\pi/4)$, then $\psi \in D(e^{ar})$ if $H\psi = E\psi$ and

$$a^2 < 2M \inf_{E_\alpha \in \sum(i\pi/4)} \{|E - \text{Re } E_\alpha| + |\text{Im } E_\alpha|\}$$

J. D. Morgan, III, in "The exponential decay of sub-continuum wave functions of two electron atoms," *J. Phys. A.* **10** (1977), L91, remarked that the bounds of Theorems XIII.39–42 cannot be the best possible, since one expects that $\psi(r)$ should asymptotically obey $H_0\psi = E\psi$ as all $r_i - r_j \to \infty$, so that one would expect that $\psi(r) \sim \exp(-\sum a_i|r_i|)$ for some a_i with $\sum a_i^2/2m_i = -E$. He has made improvements in the bounds for certain three-body systems. Large classes of N-body systems are discussed, with his remark in mind, in P. Deift, W. Hunziker, and B. Simon, "Pointwise bounds on eigenfunctions and wave packets in N-body quantum systems; IV" (to appear).

Prior to the work of O'Connor, Combes, and Thomas, there was a whole series of papers proving weaker results in different cases. One line proved that discrete eigenfunctions ψ lie in $D(r^n)$ for suitable n by using operator methods. For $n = 1, 2$ and a general class of Hamiltonians, this was proven by W. Hunziker, "Space–time behavior of Schrödinger wave functions," *J. Mathematical Phys.* **7** (1966), 300–304. This was extended to all n by J. M. Combes, "Time dependent approach to multi-channel scattering," *Nuovo Cimento* **64A** (1969), 111–144. Using a similar method, in the paper quoted above Ahlrichs proved that $\psi \in D(e^{ar})$ for atomic eigenfunctions.

A second line of attack used methods from the theory of partial differential equations. I. E. Schnoll in "On the behavior of eigenfunctions of the Schrödinger equation," *Math. Sb.* **42** (1957), 273–286 (see also the discussion in I. M. Glazman, *Direct Methods in the Qualitative*

Spectral Analysis of Singular Differential Operators, Israeli Program for Scientific Translations, Jerusalem, 1965), proved that $|\psi| \leq \exp(-ar)$, but he required his potentials to be continuous and bounded from below.

A third line employed the method of integral equations. B. Simon in his *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms*, Princeton Univ. Press, Princeton, New Jersey, 1971, proved that $\psi \in D(e^{ar})$ if $a < \sqrt{|E|}$ and $(-\Delta + V)\psi = E\psi$ with $E < 0$ and $V \in R$ (two-body case). Simon's analysis is based on a lemma in the theory of integral equations and the fact that ψ obeys

$$\psi(x) = -\frac{1}{4\pi}\int \frac{\exp(-\sqrt{-E}\,|x-y|)}{|x-y|} V(y)\psi(y)\,dy$$

For central potentials, one can use the integral equations of Section XI.8 to prove exponential falloff; see, e.g., the book by Regge and de Alfaro quoted in the Notes to Section XI.8. A final reference on the use of integral equations to prove exponential falloff is the paper of E. L. Slaggie and E. H. Wichmann, "Asymptotic properties of the wave function for a bound nonrelativistic system," *J. Mathematical Phys.* **3** (1962), 946–968, who discussed the three-body case. O'Connor's analysis is partially based on ideas from this paper.

One last line of attack uses variational methods and is described in N. W. Bazley and D. W. Fox, "Bounds for eigenfunctions of one-electron molecular systems," *Internat. J. Quant. Chem.* **3** (1969), 581–586.

Section XIII.12 The earliest results relating positivity and the nondegeneracy of an eigenvalue go back to a fundamental theorem of Perron and Frobenius: A finite matrix with strictly positive elements always has its spectral radius as an eigenvalue of multiplicity one with the corresponding eigenvector strictly positive. Notice that in the Perron–Frobenius theorem, the matrix need not be self-adjoint. The Perron–Frobenius theorem first appeared in O. Perron, "Zur theorie der Matrizen," *Math. Ann.* **64** (1907), 248–263, and F. G. Frobenius, "Über Matrizen mit positiven Elementen," *Sitzungsber. Preus. Akad. Wiss. Berlin* (1908), 471–476. The idea of extending the theorem from matrices with strictly positive elements to positivity preserving ergodic matrices appeared in F. G. Frobenius, "Über Matrizen aus nicht negativen Elementen," *Sitzungsber. Preus. Akad. Wiss. Berlin* (1912), 456–477. Further discussion of the finite matrix theorems may be found in F. Gantmacher, *Applications of the Theory of Matrices*, Wiley (Interscience), New York, 1959.

The extension of the Perron–Frobenius theorem to infinite-dimensional spaces was first accomplished by R. Jentzsch, "Über Integralgleichungen mit positiven Kernen," *J. Reine. Angew. Math.* **141** (1912), 235–244. There has been considerable development of the theory since Jentzsch's work, which dealt with a class of integral operators: See, e.g., M. Krein and M. Rutman, "Linear operators leaving invariant a cone in a Banach space," *Uspeki Mat. Nauk* **3** (1948), 3–95 [*Amer. Math. Soc. Trans.* **10** (1950), 199–235] and T. Ando, "Positive linear operators in semi-ordered linear spaces," *J. Fac. Sci. Univ. Tokyo Sect. IA Math.* **13** (1957), 214–228.

The idea of applying a theorem of Perron–Frobenius type to quantum systems is due to J. Glimm and A. Jaffe, "The $\lambda(\varphi^4)_2$ quantum field theory without cutoffs: II. The field operators and the approximate vacuum," *Ann. Math.* **91** (1970), 362–401. They used a direct proof of ergodicity for $\exp(-tH)$ where H is a spatially cutoff $P(\varphi)_2$ Hamiltonian rather than a proof going through the irreducibility of the action of $e^{-tH} \cup L^\infty(Q)$. The idea of using the irreducibility which simplifies the proof is due to I. Segal (see below). The application to nonrelativistic systems is due to B. Simon and R. Hoegh-Krohn, "Hypercontractive semi-groups and two-dimensional self-coupled Bose fields," *J. Functional Analysis* **9** (1972), 121–180. Earlier results

on nonrelativistic quantum systems which do not use the Perron–Frobenius theorem are described in R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Vol. I, Wiley (Interscience), 1953.

Theorem XIII.48 may be found in W. Faris and B. Simon, "Degenerate and non-degenerate ground states for Schrödinger operators." *Duke Math. J.* **42** (1975), 559–567.

The idea of using irreducibility in place of ergodicity goes back to Ando (see above); our proof of (c) ⇒ (a) in Theorem XIII.43 is taken from Simon–Hoegh-Krohn (see above). That the resolvent is positivity improving if it is ergodic is a theorem of Faris, "Invariant cones and uniqueness of the ground state for Fermion systems," *J. Mathematical Phys.* **13** (1972), 1285–1290. This paper also contains the perturbation theorem of Problems 91, 92. That an ergodic semigroup is positivity improving is a theorem of B. Simon, "Ergodic semigroups of positivity preserving self-adjoint operators," *J. Functional Analysis* **12** (1973), 335–339. The perturbation result, Theorem XIII.45, is due to I. Segal, "Construction of nonlinear local quantum processes, II," *Invent. Math.* **14** (1971), 211–241. The proof of statement (a) of Theorem XIII.49 is due to L. Gross, "Existence and uniqueness of physical ground states," *J. Functional Analysis* **10** (1972), 52–109. By a completely different method, Glimm and Jaffe (in the paper quoted above) had earlier proven the existence of an eigenvalue at the bottom of the spectrum of spatially cut-off $P(\varphi)_2$ Hamiltonians. We note that Theorem XIII.45 was extended to certain situations involving Fermion field theories in the Gross and Faris papers quoted above.

The Beurling–Deny criteria occur in A. Beurling and J. Deny, "Espaces de Dirichlet I. Le Cas Elementaire," *Acta Math.* **99** (1958), 203–224. The paper explicitly deals only with the case where the support of $d\mu$ is a discrete finite set with each point having mass 1. However, the proofs of what we have called the first and second Beurling–Deny criteria clearly extend to the general case (they are essentially the proofs we use)—moreover, the authors announced results for the general case although the detailed paper has never appeared! Additional discussion can be found in M. Fukushima, "On the Generation of Markov Processes by Symmetric Forms," Proc. Second Japan-USSR Symposium on Probability Theory, Lecture Notes in Mathematics, No. 336, Springer-Verlag, Berlin and New York,

Earlier than the Beurling–Deny paper, a condition closely related to their first criterion appeared in N. Aronszajn and K. T. Smith, "Characterization of positive reproducing kernels, applications to Green's functions," *Amer. J. Math.* **79** (1957), 611–622. Aronszajn and Smith discuss the question of when a strictly positive differential operator A has an inverse with a pointwise positive kernel. Their statements and, to some extent, their methods are restricted to differential operators. And their problem is slightly different from the one solved in the first Beurling–Deny criterion. For example $A = (-\Delta + 1)^2$ clearly has a positivity preserving inverse (since $A^{-1/2}$ is positivity preserving), but e^{-tA} is not positivity preserving for all $t > 0$ by the Levy–Khintchine formula. However, their condition is clearly related to the first Beurling–Deny criterion.

The first Beurling–Deny criterion provides a link between the proof we give of the nodelessness of the ground state, which relies on positivity of $e^{+t\Delta}$ and the proof we mentioned above of Courant and Hilbert. This latter proof exploits the inequality $\|\nabla|u|\|^2 \leq \|\nabla u\|^2$, which is just the first Beurling–Deny criterion for $e^{+t\Delta}$ to be positivity preserving! There is also a link between the positivity of $e^{+t\Delta}$ and Kato's inequality (Section X.4) provided by the first Beurling–Deny criterion; see B. Simon, "An abstract Kato's inequality for generators of positivity preserving semigroups." *Indiana Math. J.* (to appear).

With regard to Example 1 of Appendix 1, it is a classical theorem of T. J. Stieltjes, "Sur les Racines de l'Equation $X_n = 0$," *Acta Math.* **9** (1887), 385–400, that if A is a positive definite matrix with $a_{ij} \leq 0$ for $i \neq j$, then $(A^{-1})_{ij} \geq 0$ for all i, j. Example 1 provides a kind of converse to this theorem.

The notions in the second appendix were first introduced in a probability theory context involving infinitely divisible probability measures. All infinitely divisible probability measures with finite second moment were found by A. Kolmogorov, "Sulla forma generale di un processo stocastico omegeneo," *Atti. Accad. Naz. Lincei Rend. Cl. Sci. Fis. Mat. Natur.* **15** (1932), 805–808, 866–869. The general form was found by P. Lévy, "Sur les intégrales dont les éléments sont les variables aléatoires indépendantes," *Ann. Scuola Norm. Sup. Pisa Cl. Sci.* **3** (1934), 331–337; **4** (1935), 217–218. Further refinements are due to W. Feller, "On the Kolmogorov–P. Lévy formula for infinitely divisible distribution functions," *Proc. Yugo. Acad. Sci.* **82** (1937), 95–113, and A. Khintchine "Déduction nouvelle d'une formula de M. Paul Lévy," *Bull. Univ. d'Etat Moskov, Ser. Int. Sert A* **1** (1937), 1–5. The context in which infinitely divisible distributions enter is the following. n functions $f_1, \ldots, f_n$ on a probability measure space are called independent random variables if the measure on $\mathbb{R}^n$ given by $\nu(A) = \mu((f_1 \otimes \cdots \otimes f_n)^{-1}[A])$ is a product measure. If all the factors are the same, we say that $f_1, \ldots, f_n$ are identically distributed. If $\tilde{\mu}$ is the distribution for $f_1 + \cdots + f_n$ and μ is the one for f_i, then $\tilde{\mu} = \mu * \cdots * \mu$ (n times). If a probability distribution is a limit as $n \to \infty$ of a sum of n identically distributed random variables (the individual distribution may vary with n), then the distribution will be infinitely divisible. The classic example is that the limiting distribution be Gaussian (which corresponds to a pure $x \cdot Ax$ term in (76)). For additional discussion, see L. Breiman, *Probability*, Addison-Wesley, Reading, Massachusetts, 1968.

Conditionally positive definite functions and a theorem of the genre of Theorem XIII.52 appeared first in I. J. Schoenberg, "Metric spaces and positive definite functions," *Trans. Amer. Math. Soc.* **44** (1938), 522–536. The relation between those notions and infinitely divisible distributions has been developed by a series of Russian mathematicians: B. V. Gnedenko, "On the characteristic property of infinitely divisible distribution laws," *Bull. Mosk. Goud. Univ. Ser A.*, 1937, A. M. Yaglom and M. S. Pinsker, "Random processes with stationery nth-order increments" (in Russian), *Dokl. Akad. Nauk. SSSR* **90** (1953), 731–734; M. G. Krein, "On integral representations of Hermitian indefinite functions with a finite number of negative squares," *Dokl. Akad. Nauk. SSSR* **125** (1959), 31–34; and I. M. Gel'fand and N. Ya. Vilenkin, *Generalized Functions*, Vol. 4, Academic Press, New York, 1964. Our proof of Theorem XIII.52 follows this last presentation in part; we have corrected an error in their proof (our Theorem XIII.52; their Theorem III.4.4).

The connection between positivity preserving semigroups and the Lévy–Khintchine formula in the context of Schrödinger operator theory was made by I. Herbst and A. Sloan, "Perturbation of translation invariant positivity preserving semigroups on $L^2(\mathbb{R}^n)$," Trans. Amer. Math. Soc. (to appear), who develop some of the theory of $F(-i\nabla) + G(x)$ with F conditionally negative definite.

That $e^{-|p^4}$ does not generate a positivity preserving semigroup has been used to construct an example illustrating the difference between different axiom schemes for Euclidean quantum field theories; see B. Simon, "Positivity of the Hamiltonian semigroup and the construction of Euclidean region fields," *Helv. Phys. Acta* **46** (1973), 686–696.

Section XIII.13 The potential constructed in Example 1 is due to J. von Neumann and E. P. Wigner, "Über merkwürdige diskrete Eigenwerte," *Z. Phys.* **30** (1929), 465–467. There is an arithmetic mistake in their paper, so that the potential they write down has $O(r^{-2})$ behavior at infinity violating Theorem XIII.58. We have corrected their arithmetic mistake. Unaware of their work, J. Weidmann in "Zur Spektraltheorie von Sturm–Liouville Operatoren," *Math. Z.* **98** (1967), 268–302 constructed an example using step functions (much in the spirit of Nelson's example discussed in Example 1 of the Appendix to Section X.1). S. Albeverio in "On bound states in the continuum of N-body systems and the Virial theorem," *Ann. Phys.* **71** (1972),

167–276, describes how one can construct potentials with bound states at any finite number of prescribed energies. See also the Atkinson paper quoted in the Notes to Section XI.8.

Theorems in the genre of Theorem XIII.56 are to some extent implicit in the work on Jost functions and solutions discussed in Section XI.8. In particular, the inverse scattering techniques discussed in the Notes to that section are critical in the Albeverio construction quoted above. Explicit theorems exploiting ordinary differential equation techniques to completely analyze the spectrum of operators with central potentials, and, in particular, results stronger than Theorem XIII.56 or the central case of Theorem XIII.58, appear in Weidmann's paper above. For additional discussion of Jost function techniques and positive energy bound states, see the appendix to Section XI.8 and its Notes.

The model for Theorem XIII.58 is a paper of F. Rellich, "Über das asymptotische Verhalten der Lösungen von $\Delta u + \lambda u = 0$ in unendlichen Gebieten," *Über. Deutsch. Math. Verein* **53** (1943), 57–65. Rellich studied solutions of $(\Delta + \lambda)u = 0$ in unbounded domains and in particular proved that there are no square integrable solutions of $(\Delta + \lambda)u = 0$ in $\mathbb{R}^n \setminus \{x \mid |x| > R\}$ if $\lambda > 0$. This implies that there are no positive eigenvalues of $-\Delta + V$ if V has compact support. This idea was developed by T. Kato, "Growth properties of solutions of the reduced wave equation with variable coefficients," *Comm. Pure Appl. Math.* **12** (1959), 403–425, who proved the case of Theorem XIII.52 with $V_2 = 0$. Results proven by similar means for potentials that are repulsive near infinity ($\partial V_2/\partial r < 0$ for r large) can be found in K. Kreith, "Differential operators with a purely continuous spectrum," *Proc. Amer. Math. Soc.* **14** (1963), 809–811, and F. Odeh, "Note on differential operators with a purely continuous spectrum," *Proc. Amer. Math. Soc.* **16** (1965), 363–366. Theorems of the form of Theorem XIII.58 (but with slightly stronger smoothness conditions) were found independently by B. Simon, "On positive eigenvalues of one-body Schrödinger operators," *Comm. Pure Appl. Math.* **22** (1969), 531–538, and S. Agmon, "Lower bounds for solutions of Schrödinger-type equations in unbounded domains," *Proceedings of the International Conference on Functional Analysis and Related Topics*, 1969, Univ. Tokyo Press, Tokyo, and "Lower bounds for solutions of Schrödinger equations," *J. Analyse Math.* **23** (1970), 1–25. Even before these later papers, J. Weidmann, "On the continuous spectrum of Schrödinger operators," *Comm. Pure Appl. Math.* **19** (1966), 107–110, used the methods from Kato's paper to show that Coulombic Hamiltonians have no positive eigenvalues (this was the first proof of this result which we discuss in Example 5 and Example 5 (revisited) using other techniques). Weidmann's methods easily extend to homogeneous potentials of degree $-\alpha$, $0 < \alpha < 2$. In the second Agmon paper, sums of potentials of the type considered in Theorem XIII.58 and these homogeneous potentials are discussed. The techniques of Theorem XIII.58 are extended to systems with magnetic fields in T. Ikebe and J. Uchiyama, "On the asymptotic behavior of eigenfunctions of second order elliptic operators," *J. Math. Kyoto Univ.* **11** (1971), 425–448. Applications of the method to assert that certain special classes of n-body operators have no eigenvalues in (E_0, ∞) for suitable $E_0 > 0$ can be found in the Simon paper and the first Agmon paper.

In the physics literature the statement of the virial theorem in quantum mechanics goes back to B. N. Finkelstein, "Über den Virialsatz in der Wellenmechanik," *Z. Phys.* **50** (1928), 293–294. Finkelstein used the formal commutator we describe in the text. While it was clear to Weidmann (who gave the first rigorous proof of the virial theorem; see below) that making Finkelstein's proof rigorous presented problems, it was Albeverio in the paper quoted above who emphasized that there were modifications of the Wigner–von Neumann example with wave functions not in the domain of the dilation generator D. Nevertheless, H. Kalf in "The quantum mechanical virial theorem and the absence of positive energy bound states of Schrödinger operators," *Israel J. Math.* **20** (1975), 57–69, did find a proof of the virial theorem along Finkelstein's lines. Essentially, the commutator argument is replaced by an explicit integration

by parts. The bad domain properties imply that the boundary terms in the integration by parts do not automatically go to zero and they must be treated by a careful averaging argument.

The connection of the virial theorem and the group of dilations is a discovery of V. Fock, "Bemerkung zum Virialsatz," *Z. Phys.* **63** (1930), 855–858. The first rigorous proof of the virial theorem, which we follow in our proof, is due to J. Weidmann, "The virial theorem and its application to the spectral theory of Schrödinger operators," *Bull. Amer. Math. Soc.* **73** (1967), 452–456. Weidmann also discovered the relevance of the virial theorem to the problem of positive eigenvalues. Virial theorem techniques are further discussed in Albeverio's paper, which includes an extension to operators with magnetic fields, and Kalf's paper which includes the case of certain operators defined as sums of quadratic forms.

The application of dilation analytic techniques to recover Weidmann's theorem on the nonexistence of positive eigenvalues for Coulombic Hamiltonians was first noted in B. Simon, "Resonances in N-body quantum systems with dilation analytic potentials and the foundations of time dependent perturbation theory," *Ann. Math.* **97** (1973), 247–274. Simon also remarked that spherically symmetric dilation analytic potentials automatically have $r\,dV/dr \to 0$ at infinity so that, on the basis of Theorem XIII.83, one might expect connections between dilation analytic potentials and the lack of positive energy eigenvalues. Our discussion in Example 5 (revisited) does not follow Simon's paper but rather an unpublished remark of E. Balslev. The argument in Example 5, revisited, alternate argument, is due to W. Hunziker, "The Schrödinger Eigenvalue problem for N-particle systems," in *The Schrödinger Equation*, (W. Thirring and P. Urban, eds.) Springer, 1977, 43–72.

Carlson's theorem was proven by F. Carlson in his 1914 University of Upsala Thesis. He also proved the beautiful corollary on continuing an analytic function from its values at the positive integers (see Problem 109). Theorem XIII.61 was proven independently by B. Simon, "Absence of positive eigenvalues in a class of multiparticle quantum systems," *Math. Ann.* **207** (1974), 133–138, and E. Balslev, "Absence of Positive Eigenvalues of Schrödinger Operators," *Arch. Rational Mech. Anal.* **59**, 4 (1975), 343–357.

Unique continuation theorems were first proven for operators of second order on $\mathbb{R}^2$ by T. Carleman, "Sur un probleme d'unicité pour les systèmes d'équations aux dérivées partielles à deux variables indépendantes," *Ark. Mat.* (17) **26B** (1939), 1–9. Carleman introduced the idea, which is critical in our proof, of proving a priori estimates with constants independent of a parameter (β in our case), so that as the parameter becomes singular, the integrals in the estimates become more and more concentrated in some region of interest. Unique continuation for Schrödinger operators in n-dimensions was first proven by C. Müller, "On the behavior of the solutions of the differential equation $\Delta u = F(x, u)$ in the neighborhood of a point," *Comm. Pure Appl. Math.* **7** (1954), 505–515. This problem was further studied by E. Heinz, "Über die Eindeutigkeit beim Cauchyschen Anfangswertproblem einer elliptischen Differentialgleichung zweiter Ordnung," *Nachr. Akad. Wiss. Göttingen Math.-Phys. Kl. II* (1) (1955), 1–12, whose proof we follow in the appendix to this section. Heinz, in particular, proved a unique continuation theorem for Schrödinger operators with magnetic fields (see Problem 113). These results were extended to second-order elliptic equations with nonconstant leading coefficients independently by N. Aronszajn, "A unique continuation theorem for solutions of elliptic partial differential equations or inequalities of second order," *J. Math. Pures Appl.* **36** (1957), 235–249, and H. O. Cordes, "Über die Bestimmtheit der Lösungen ellipticher Differentialgleichungen durch Anfangsvorgaben," *Nachr. Akad. Wiss. Göttingen Math.-Phys. Kl. II* (11) (1956), 239–258.

For hyperbolic equations like the wave equation $\ddot{u} = \Delta u$, it can happen, of course, that solutions can vanish in open sets without being identically zero, but there is a uniqueness theorem in this case also: If $\ddot{u} = \Delta u$ and u vanishes in some neighborhood of the plane $\{(t, \mathbf{x}) \mid t = 0\}$, then u is identically zero. For the wave and related equations, such results go back at least to E. Holmgren, "Über Systeme von linearen partiellen Differentialgleichungen," *Öfver-*

sigt af Kongl. Vetenskaps-Akad. Förh. **58** (1901), 91–105; see also L. Nirenberg, "Uniqueness in Cauchy problems for differential equations with constant leading coefficients," *Comm. Pure Appl. Math.* **10** (1957), 89–105, and A. P. Calderón, "Uniqueness in the Cauchy problem for partial differential equations," *Amer. J. Math.* **80** (1958), 16–36. These results are discussed in detail in the book by L. Hörmander, *Linear Partial Differential Operators*, Springer-Verlag, Berlin and New York, 1964. There are examples of operators with no uniqueness theorem constructed by P. Cohen, "The non-uniqueness of the Cauchy Problem," O.N.R. Technical Report 93, Stanford, 1960 and A. Pliv, "A smooth linear elliptic differential equation without any solution in a sphere," *Comm. Pure Appl. Math.* **14** (1961), 599–617.

As emphasized by R. Lavine (unpublished), there is a serious defect in the unique continuation theorems that are available in that they require that V be bounded locally. The kind of "trapping" that occurs in Example 2 has a potential V that is not even locally L^1 and the theorem of Faris and Simon (Theorem XIII.48) suggests strongly that such non-L^1 singularities are necessary for trapping. For example, one would conjecture: If $V \in L^1_{\text{loc}}(\mathbb{R}^n)$ is positive and $H = -\Delta + V$ is defined as a sum of forms, then any eigenfunction of H vanishing on an open set is identically zero. Notice that Heinz's proof throws away a lot of information in the estimates. By carefully keeping track of this information, one should be able to prove a unique continuation theorem for certain classes of unbounded potentials.

In the application that we make of unique continuation, we only need the special case which prohibits eigenfunctions of compact support. This fact has been proven in greater generality using Theorem XIII.100 by W. O. Amrein and A. Berthier, to appear.

Section XIII.14 The basic criterion, Theorem XIII.64, and the other general results of this section (Theorems XIII.77, 78) are standard folklore. Theorem XIII.78 was first emphasized in a mathematical physics context by J. Glimm and A. Jaffe, "The $\lambda(\varphi^4)_2$ quantum field theory with cutoffs II. The field operators and the approximate vacuum," *Ann. Math.* **91** (1970), 362–40, who applied it to the spatially cutoff $P(\varphi)_2$ Hamiltonian. An application to the spatially cutoff Y_2 model and the proof we use via Theorem XIII.77 appears in their paper, "The Yukawa$_2$ Quantum Field theory without cutoffs," *J. Functional Analysis* **7** (1971), 323–357.

We have decided to call Theorem XIII.65 Rellich's criterion because the earliest related results appeared in F. Rellich, "Ein Satz über mittlere Konvergenz," *Nachr. Akad. Wiss. Göttingen Math.-Phys. Kl. II* (1930), 30–35. The authors learned the simple proof given in the text from R. Lavine.

Riesz' criterion appeared in M. Riesz, "Sur les ensembles compacts de fonctions sommable," *Acta Sci. Math.* (*Szeged*) **6** (1933), 136–142. Earlier related results are due to M. Fréchet, "Essai de geometrie analytique à une infinité de coordinates," *Nouvelles Ann. Math.* **8** (1903), 97–116; 289–317, and A. Kolmogoroff," Über Kompaktheit der Funktionmengen bei der Konvergenz im Mittel," *Nachr. Akad. Wiss. Göttingen Math.-Phys. Kl. II* (1931), 60–63.

Our discussion of the falloff of eigenfunctions of $-\Delta + V$ with $V \to \infty$ is taken from B. Simon, "Pointwise bounds on eigenfunctions and wave packets in N-body quantum systems, I, II, III," *Proc. Amer. Math. Soc.* **42** (1974), 395–401; **45** (1974), 454–456; *Trans. Amer. Math. Soc.* **208** (1975), 317–329. In particular, a proof of Theorem XIII.72 can be found in the paper III. Theorem XIII.70, in the $V \geq 0$ case, appeared much earlier in I. Schnol, "On the behavior of the eigenfunctions of Schrödinger's equation," *Mat. Sb.* **46** (88) (1957), 273–286, *erratum* 259; where it was proven by different means. Our proof of Theorem XIII.70 in the $V \geq 0$ case uses a trick of E. B. Davies, "Properties of the Green's functions for some Schrödinger operators," *J. London Math. Soc.* **7** (1973), 483–491. Extensions of Theorem XIII.72b to say something about eigenfunctions other than the ground state occur in C. Bardos and M. Merigot, "Asymptotic decay of the solution of a second order elliptic equation in an unbounded domain. Applications to the

spectral properties of a Hamiltonian," *Proc. Roy. Soc. Edinburgh Sect. A* (to appear), and C. Bardos and M. Merigot, "Décroissance expontielle de la solution L^2 du problème de Dirichlet dans le complementaire d'un fermé borné," *Comp. Rend. Acad. Sci. Paris*, **281A** (1975), 561–563.

The first compact embedding theorem of the type we discuss was proved by F. Rellich in the paper quoted above. General embedding theorems for H_0^m are due to L. Gårding, "Dirichlet's problem for linear elliptic partial differential equations," *Math. Scand.* **1** (1953), 55–72. Gårding's proof is outlined in Problem 123. Rellich proved Theorem XIII.75 in the case of bounded regions with smooth boundary. The general case and the theory of regions obeying the segment property is due to S. Agmon, *Lectures on Elliptic Boundary Value Problems*, Van Nostrand, Princeton, New Jersey, 1965. Agmon also proves that if Ω has the segment property, then $\{f \mid f$ is C^∞ in a neighborhood of $\Omega\}$ is dense in H^m.

Our discussion of quantum statistical mechanics in boxes is taken from B. Simon's appendix to J. Lebowitz and E. Lieb, "The constitution of matter," *Advances in Math.* **9** (1972), 316–398, but the subject is fairly standard folklore. For further discussion of the quantum statistical mechanics of continuous systems, see J. Ginibre, "Some applications of Functional Integration in Statistical Mechanics" in *Statistical Mechanics and Quantum Field Theory, Les Houches, 1970* (C. DeWitt and R. Stora, eds.) Gordon and Breach, New York, 1971, D. Robinson, *The Thermodynamic Pressure in Quantum Statistical Mechanics*, Springer-Verlag, Berlin and New York, 1971, and D. Ruelle, *Statistical Mechanics*, Benjamin, New York, 1967.

Section XIII.15 The technique of Dirichlet–Neumann bracketing is one with a considerable antiquity; for example, Theorem XIII.78 is proven in R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Vol. I, Wiley (Interscience), 1953, see especially pp. 429–431, by a method related to Dirichlet–Neumann bracketing. Weyl's original proof uses related ideas. More recent papers employing the method are E. H. Lieb, "Quantum Mechanical Extensions of the Lebowitz–Penrose Theorem on the Van Der Waals Theory," *J. Mathematical Phys.* **7** (1966), 1016–1024, and A. Martin, "Bound states in the strong coupling limit," *Helv. Phys. Acta* **45** (1972), 140–148, and the book by Robinson quoted in the Notes to the last section.

For arbitrary open regions $\Omega \subset \mathbb{R}^m$ one can choose different definitions for $-\Delta_N$ than the one we gave. For example, some authors take $Q(-\Delta_N)$ to be the closure of the form $(f, -\Delta f)$ on the set of functions in $H^1(\Omega)$ which are C^∞ in a neighborhood of Ω. For regions that obey the segment condition, the definitions agree.

The intuitive idea that one state takes up a volume h^3 in phase space entered quite early in attempts to extend Bohr's old quantum theory to gases; see, for example, O. Sackur, "Die Anwendung der Kinetischen Theorie der Gase auf chemische Probleme," *Ann. Phys.* **36** (1911), 958–980; "Die universelle Bedeutung des sog. elementaren Wirkungsquantums," *Ann. Phys.* **40** (1913), 67–86; and H. Tetrode, "Die chemische Konstante der Gase und das elementare Wirkungsquantum," *Ann. Phys.* **38** (1912), 434–442. This idea was used as a powerful tool by E. Fermi even after the development of the new quantum theory and is called the "Fermi gas picture."

Finding the number of points of $\mathbb{Z}^m$ inside the ball of radius r is of considerable number-theoretic interest. That the number is asymptotically $\tau_m r^m$ with an error at worst $O(r^{m-1})$ is a result going back at least to Gauss who used a proof which is essentially that used in Proposition 2. Surprisingly, the error is smaller than $O(r^{m-1})$ in fact, for $m = 2$ it is known to be smaller than $O(r^{2/3})$ and larger than $O(r^{1/2})$. For further discussion, see §18.7 of G. Hardy and E. Wright, *The Theory of Numbers*, Oxford Univ. Press, Oxford, 1938, and pages 183–308 of E. Landau, *Vorlesungen über Zahlen Theorie*, Vol. 2, Hirzel, Leipzig, 1927. For the analogous problem in higher dimensions, see A. Walfisz, *Weylische Exponentialsummen in der Neueren Zahlentheorie*, Deutscher Ver. Wiss., Berlin, 1963. We warn the reader that these results do not

imply that the power $m-1$ in (116) and (117) can be improved. Quite the contrary, they imply that it cannot be improved! For the set M_{m-1} will make a contribution of order r^{m-1}, which by the above cannot be made up for by the contribution of the surface of the ball.

Theorem XIII.78 is a celebrated theorem of H. Weyl, "Das asymptotische Verteilungsgesetz der Eigenwerte linearer partieller Differentialgleichungen," *Math. Ann.* **71** (1911), 441–469, and "Über die Abhänggigkeit der Eigenschwenkgungen einer Membran von deren Begrenzung," *J. Math.* **141** (1912), 1–11. For a historical reminiscence, see H. Weyl, "Ramifications, old and new, of the eigenvalue problem," *Bull. Amer. Math. Soc.* **56** (1950), 115–139. This theorem has captured the imagination of two generations of mathematicians. Weyl's work was based on conjectures of Lorentz and Jeans who came upon the problem in the study of electromagnetic radiation theory. It shows that the spectrum of $-\Delta_\Omega$ on Ω determines the volume of Ω. This immediately raises the question of what other geometric properties of Ω are determined by the spectrum of $-\Delta_\Omega$, or more generally the Laplace–Beltrami operator on a compact Riemannian manifold $-\Delta_M$. The results up until the middle 1960s and important new directions are summarized in the beautiful article of M. Kac, "Can you hear the shape of a drum," *Amer. Math. Monthly* (Slaught Memorial Papers, No. 11) (4) **73** (1966), 1–23. More recent results are discussed in I. M. Singer's contribution to the Proceedings of the 1974 International Congress of Mathematicians entitled "Distribution of eigenfrequencies for the Laplacian." See also, R. Ballian and C. Bloch, "Eigenvalues of wave equation in a finite domain, I, II, III;" *Ann. Phys.* **60** (1970), 401; **64** (1971), 271; **69** (1972), 75. Among the things determined by the eigenvalues are the surface area of the boundary, the Euler–Poincaré characteristic, and the lengths of any closed geodesics on M. On the negative side is the existence of an example given by J. Milnor in "Eigenvalues of the Laplacian operator on certain manifolds," Proc. *Nat. Acad. Sci.* **51** (1964), 542, of two nonisometric 16-dimensional tori whose Laplace–Beltrami operators have identical spectra. These analyses of $-\Delta_\Omega$ rely on studying the integral kernel for $\exp(t\Delta_\Omega)$ rather than on the method of Dirichlet–Neumann bracketing, which is too crude to see anything but the leading term in $N(\lambda)$. A modern discussion of these Green's functions methods can be found in L. Hormander, "The spectral function of an elliptic operator," *Acta Math.* **121** (1968), 193–218.

For certain regions one can show that the error in Weyl's formula is $O(\lambda^{(n-1)/2})$; See the Hörmander paper quoted above and V. Avakumovic, "Über die Eigenfunctionen auf geschlossen Riemannschen Mannigfaltigkeiten," *Math. Z.* **65** (1956), 327–344.

For an example where a phase space picture provides a bound on a quantum-mechanical situation, see Theorem XIII.12 and Problems 31, 32, 33. We remark that while the phase space volume picture is remarkably accurate in most situations, it does fail in "borderline" situations. For example, $-\Delta - c(1+|r|)^{-\alpha}$ on $L^2(\mathbb{R}^3)$ has an infinite number of bound states if $\alpha < 2$, $c > 0$ or $\alpha = 2$, $c > \frac{1}{4}$. The negative energy phase space volume is infinite whenever $\alpha \leq 2$, $c > 0$. Thus for $\alpha = 2$, $0 < c \leq \frac{1}{4}$, the phase space prediction is wrong.

Jordan content was an important precursor of Lebesgue measure. The basic work was done in the 1880s by Cantor, Stolz, Harnack, Peano, and Jordan. A historical discussion of the development of content can be found in I. N. Pesin, "Classical and Modern Integration Theories," Academic Press, New York, 1970. Modern treatments of Jordan content occur in L. Loomis and S. Sternberg, *Advanced Calculus*, Addison-Wesley, Reading, Massachusetts, 1968, and T. Apostol, *Mathematical Analysis*, Addison-Wesley, Reading, Massachusetts, 1960.

Theorem XIII.79 (in slightly different forms) is due to M. S. Birman and V. V. Borzov, "On the asymptotics of the discrete spectrum of some singular differential operators," *Probs. Math. Phys.* **5** (1971), 24 (*Topics Math. Phys.* **5** (1972), 19–30), A. Martin (the paper quoted above), and H. Tamura, "The asymptotic eigenvalue distribution for non-smooth elliptic operators," *Proc. Japan Acad.* **50** (1974), 19–22. Earlier, K. Chadam, in "The asymptotic behavior of the number of bound states of a given potential in the limit of large coupling, II," *Nuovo Cimento* **58A**

(1968), 191–204, had proven a similar result for one-dimensional systems and B. Simon, "On the growth of the number of bound states with increase of potential strength," *J. Mathematical Phys.* **10** (1969), 1123–1126 had proven $c\lambda^{3/2} < N(\lambda) < d\lambda^{3/2}$ for λ large; $c, d > 0$; $n = 3$. Martin uses Dirichlet–Neumann bracketing, Chadam uses Jost function methods (see Section XI.8), and Tamura uses Green's function methods. Extensions and further development may be found in a set of papers by Birman and co-workers: M. S. Birman and M. E. Solomjak, "Piece-wise polynomial approximations of functions of the classes W_p^α," *Math. Sb.* **73** (1967), 331–355 (*Math. USSR Sb.* **2** (1967), 295–313), "On the leading term in the asymptotic spectral formula for non-smooth elliptic problems," *Funckcional Anal. i Priložen* (4) **4** (1970), 1–14 [*Functional Anal. Appl.* **4** (1970), 265–275], "On the asymptotic spectrum of non-smooth elliptic equations," *Funkcional Anal. i Priložen* (1) **5** (1971), 69–70 [*Functional Anal. Appl.* **5** (1971), 56–58]; V. V. Borzov, "On some applications of piece-wise polynomial approximations of functions of anisotropic classes W_p^r," *Dokl. Akad. Nauk SSSR* **198** (1971), 499–501 [*Soviet Math. Dokl.* **12** (1971), 804–807]; G. V. Rosenbljum, "On the distribution of eigenvalues of the first boundary value problem in unbounded domains," *Dokl. Akad. Nauk SSSR* **200** (1971), 1034–1036 [*Soviet Math. Dokl.* **12** (1971), 1539–1542].

The method of proof of Theorem XIII.80 is due independently to Birman, in the paper quoted above, and to Simon in the weak trace ideal paper quoted in the Notes to Section 3.

One can also prove limit theorems on the quantities $S_\gamma(V)$ of Problem 32 and use the Lieb–Thirring bounds to extend them to arbitrary potentials in $L^{m/2+\gamma}$ (see Problems 129 and 130).

Variants of Theorem XIII.81 appear in E. C. Titchmarsh's books, *Eigenfunction Expansions, Parts I, II*, Oxford Univ. Press, London and New York, Part I, 2nd ed., 1962; Part II, 1958.

Variants of Theorem XIII.82 appear in F. H. Brownell and C. W. Clark, "Asymptotic distribution of the eigenvalues of the lower part of the Schrödinger operator spectrum," *J. Math. Mech.* **10** (1961), 31–70, and J. B. McLeod, "The distribution of eigenvalues for the hydrogen atom and similar cases," *Proc. London Math. Soc.* **11** (1961), 139–158. Generalizations to other operators appear in H. Tamura, "The asymptotic distribution of the lower part eigenvalues for elliptic operators," *Proc. Japan Acad.* **50** (1974), 185–187.

Extensions of Theorem XIII.82 to various multiparticle systems may be found in Simon's "Geometric methods" paper quoted in the Notes to Section 3.

Applications of Dirichlet–Neumann bracketing to quantum statistical mechanics can be found in D. Robinson, *The Thermodynamic Pressure in Quantum Statistical Mechanics*, Springer-Verlag, Berlin and New York, 1971; to the Fock space energy per unit volume in quantum field theory in F. Guerra, L. Rosen, and B. Simon, "Boundary conditions for the $P(\varphi)_2$ euclidean quantum field theory," *Ann. Inst. H. Poincaré* **25A** (1976), 231–334, and to the Thomas–Fermi model in E. Lieb and B. Simon, "The Thomas–Fermi model of atoms, molecules and solids," *Advances in Math.* **23** (1977), 22–116.

Theorems of the genre of Theorem XIII.82.5 go back at least to the Titchmarsh books quoted above and have been extended to more general potentials. The result is sometimes expressed in the form

$$\sqrt{E_n(V)} = n\pi + \frac{1}{2\pi} n^{-1} \int_0^1 V(x)\, dx + o(n^{-1})$$

By the remarks after the theorem, if V is sufficiently smooth (C^1 is enough), the error will be $o(n^{-2})$.

Section XIII.16 The theory of direct integrals is more general than what we discuss in that nonconstant fibers are allowed. In the case where all fibers are separable, every direct

integral over M is unitarily equivalent to one of the following by a unitary which is a fibered map: Let $M = M_\infty \cup (\bigcup_{n=1}^{\infty} M_n)$ where $M_\infty, M_1, \ldots$ are disjoint measurable sets. Let

$$\mathscr{H} = \int_{M_\infty}^{\oplus} \ell_2 \oplus \left(\bigoplus_{n=1}^{\infty} \int_{M_n}^{\oplus} \mathbb{C}^n \right)$$

in terms of our constant fiber direct integrals. Direct integrals were introduced and developed by J. von Neumann, "On rings of operators: Reduction theory," *Ann. Math.* **50** (1949), 401–485. Von Neumann used his theory to decompose weakly closed algebras of operators as direct integrals of factors (see Chapter XVIII). For further discussion and references, see J. Dixmier, *Les Algèbras d'opérateurs dans l'espace Hilbertien*, Chapter II, Gauthier-Villars, Paris, 1969.

While the analysis of differential operators with periodic coefficients did not mention direct integral theory until relatively recently, the key notion that solutions should be analyzed by looking for solutions on $\mathbb{R}$ (or $\mathbb{R}^n$) which are not periodic but obey $\psi(x + a) = e^{i\theta}\psi(x)$ is an early one. It was realized in the mathematical literature by G. Floquet, and in the solid state physics literature by F. Bloch, "Über die Quantenmechanik der Elektronen in Kristallgittern," *Z. Phys.* **52** (1928), 555–600.

There is an enormous mathematical literature on ordinary differential equations with periodic coefficients, especially *Hill's equation*, $(P(x)y'(x))' + Q(x)y(x) = \lambda y(x)$ with P and Q having a common period. Books on the subject include W. Magnus and S. Winkler, *Hill's Equation*, Wiley (Interscience), 1966; M. S. P. Eastham, *The Spectral Theory of Periodic Differential Equations*, Scottish Academic Press, 1973; and parts of E. A. Coddington and N. Levinson, *Theory of Ordinary Differential Equations*, McGraw-Hill, New York, 1955; and E. C. Titchmarsh, *Eigenfunction Expansions, Parts I, II*, Oxford Univ. Press, London and New York, 1962 (2nd ed.), 1958.

The analysis of the discriminant is normally based on direct ordinary differential equation methods rather than analytic perturbation theory, see, for example, Eastham's book. The results go back to work of Liapunov, "Problème generale de la stabilité du movement," *Ann. Fac. Sci. Toulouse* (2) **9** (1907), 203–474, G. Hamel, "Über die lineare Differentialgleichungen zweiter ordnung mit periodischen Koeffizienten," *Math. Ann.* **73** (1913), 371–412; O. Haupt, "Über lineare homogene Differentialgleichungen 2. ordnung mit periodischen Koeffizienten," *Math. Ann.* **79** (1919) 278–285; and H. A. Kramers, "Das Eigenwertproblem in eindimensionalen periodischen Kraftfeldern," *Physica* **2** (1935), 483–490.

The fact that the Mathieu equation has all its gaps is due to E. L. Ince, "A proof of the impossibility of the coexistence of two Mathieu functions," *Proc. Cambridge Phil. Soc.* **21** (1922), 117–120. The example in Problem 139 has been analyzed by R. L. Krönig and W. G. Penny, "Quantum mechanics in crystal lattices," *Proc. Roy. Soc.* **130** (1931), 499–513, and is a common pedagogical model in solid state physics. Theorem XIII.91 (a) and (c) are due to G. Borg, "Eine Umkehrung der Sturm–Liouvilleschen eigenwertaufgabe Bestimmung der Differentialgleichung durch die Eigenwerte," *Acta Math.* **78** (1946), 1–96. Alternative proofs of (a) can be found in H. Hochstadt, "On the determination of a Hill's equation from its spectrum, I," *Arch. Rational Mech. Anal.* **19** (1965), 353–62; H. Hochstadt, "Function theoretic properties of the discriminant of Hill's equation," *Math. Z.* **82** (1963), 237; and P. Ungar, "Stable Hill equations," *Comm. Pure Appl. Math.* **14** (1961), 707–710. The first quoted Hochstadt paper contains a proof of (b) and the statement (d′) obtained by replacing real analytic by C^∞. An alternative proof of (c) can be found in H. Hochstadt, "On the determination of a Hill's equation from its spectrum, II," *Arch. Rational Mech. Anal.* **23** (1966), 237–238. (d) is due to W. Goldberg, "On the determination of a Hill's equation from its spectrum," *Bull. Amer. Math. Soc.* **80** (1974),

1111–1112 and H. P. McKean and E. Trubowitz, "Hill's equation and hyperelliptic function theory in the presence of infinitely many branch points," *Comm. Pure Appl. Math.* **29** (1976), 143–226.

This later paper also contains (e), Theorem XIII.92, and the $n = \infty$ case of Theorem XIII.94. (e) is independently due to B. Simon, "On the genericity of non-vanishing instability intervals in Hill's equation," *Ann. Inst. H. Poincaré* **24A** (1976), 91–93. The $n < \infty$ case of Theorem XIII.94 occurs in H. P. McKean and P. van Moerbeke, "The spectrum of Hill's equation," *Invent. Math.* **30** (1975), 217–274. Theorem XIII.93 is due to C. Gardner, J. Greene, and M. Kruskal and R. Muira, "A method for solving the Korteweg de Vries equation," *Phys. Rev. Lett.* **19** (1967), 1095–1097. In comparison with (d) of Theorem XIII.91, Eastham remarked in his book that for periodic Schrödinger operators on $\mathbb{R}^m$ with $m \geq 2$, there are finitely many gaps for suitable potentials which are not even continuous.

The reader can find Hadamard's factorization theorem in E. C. Titchmarsh, *Function Theory*, Cambridge Univ. Press, London and New York, 1939. Theorem XIII.95 is due to W. Kohn, "Analytic properties of Bloch waves and Wannier functions," *Phys. Rev.* **115** (1959), 809–821. Additional discussion of this theorem and the analyticity of band functions can be found in J. Avron and B. Simon, "Analytic properties of band functions" *Ann. Phys.* (1977).

Theorem XIII.96 on uniformly local estimates is due to R. Strichartz, "Multipliers on fractional Sobolev Spaces," *J. Math. Mech.* **16** (1967), 1031–1060.

Basic papers on the spectral analysis of N-dimensional periodic Schrödinger operators are F. Odeh and J. B. Keller, "Partial differential equations with periodic coefficients and Bloch waves in crystals," *J. Mathematical Phys.* **5** (1964), 1499–1504; G. Scherf, "Das Blochsche Theorem für unendliche Systeme," *Helv. Phys. Acta* **39** (1966), 556–560; J. Avron, A. Grossman, and R. Rodrijuez, "Hamiltonians in the one-electron theory of solids," *Rep. Mathematical Phys.* **5** (1974), 113–120; L. E. Thomas, "Time dependent approach to scattering from impurities in a crystal," *Comm. Math. Phys.* **33** (1973), 335–343 and G. M. Troiuniellog, "Scattering theory for Schrödinger operators with L^∞ potentials and distorted Bloch waves," *J. Mathematical Phys.* **15** (1974), 2048–2052; F. Bentosela, "Scattering from impurities in a crystal," *Comm. Math. Phys.* **46** (1976), 153–166. Thomas' paper, in particular, contains the clever argument ((c) of the lemma to Theorem XIII.100) showing that no function $E_n(z)$ is constant and the resulting Theorem XIII.102. Thomas actually handles the case $\beta = 2$ for $n = 3$.

The eigenfunction expansion of Theorem XIII.98 is due to I. M. Gel'fand, "Expansion in series of eigenfunctions of an equation with periodic coefficients," *Dokl. Akad. Nauk SSSR* **73** (1950), 1117–1120.

There are rather subtle spectral properties of periodic Hamiltonians in electric and magnetic fields; see, e.g., A. Grossman, "Momentum-like constants of motion" in *Statistical Mechanics and Field Theory*, (R. N. Sen and C. Weil, eds.) Halsted Press, Washington, D.C., 1972.

The model of impurities that we discussed at the conclusion of this section is unrealistic in the sense that single impurity atoms do not occur but rather a low density of impurity atoms distributed randomly. There is an interesting model of this situation. Let V and W be two potentials on $[0, 1)$. Let z denote a two sided sequence $\{z_n\}$, $n = 0, \pm 1, \pm 2, \ldots$, of 0 and 1. Given z, let $V^{(z)}$ be the function on $\mathbb{R}$ that is $V(x - n)$ on $[n, n + 1)$ if $z_n = 0$ and $W(x - n)$ if $z_n = 1$. Let $H^{(z)} = -d^2/dx^2 + V^{(z)}(x)$ as an operator on $L^2(\mathbb{R})$. Let p be the density of impurities. On $\{0, 1\}^{\mathbb{Z}}$, put the product measure with $\mu(\{0\}) = 1 - p$; $\mu(\{1\}) = p$ on each factor. One now thinks of $H^{(z)}$ as a "random Hamiltonian" and asks about properties that hold for almost every $H^{(z)}$. One can prove that almost every $H^{(z)}$ has a complete set of eigenvectors! See Goldshade and Molchanov, "On the Mott's problem," *Dokl. Akad. Nauk SSSR* **230** (1976), 761–764.

Good references for elementary solid state theory are C. Kittel, *Quantum Theory of Solids*, Wiley, New York, 1963, and Ziman, *Principles of The Theory of Solids*, Cambridge Univ. Press, London and New York, 1972.

Section XIII.17 We have discussed only one aspect of the spectral theory of non-self-adjoint operators. Among the places where the reader can look for additional material are I. C. Gohberg and M. G. Krein, *Introduction to the Theory of Linear Non-self-adjoint Operators*, Amer. Math. Soc. Transl., Vol. 18, 1969 (Russian original 1965), and *Theory and Applications of Volterra Operators in Hilbert space*, Amer. Math. Soc. Translations, Vol. 24, 1970; I. C. Gohberg and I. A. Feldman, *Convolution Equations and Projection Methods for Their Solution*, Amer. Math. So. Transl., 1974; R. Douglas, *Banach Algebra Techniques in Operator Theory*, Academic Press, New York, 1972; N. Dunford and J. Schwartz, *Linear Operators*, Part II, Sections XI.6, 9, 10, Wiley (Interscience), 1963; B. Sz. Nagy and C. Foias, *Harmonic Analysis of Operators on Hilbert Space*, North Holland, Amsterdam, 1970, and *Proceedings of a Conference on Operator Theory*, Lecture Notes in Mathematics No. 345, Springer-Verlag, Berlin and New York, 1973; C. Pearcy (ed.), *Topics in Operator Theory*, Amer. Math. Soc., Providence, Rhode Island, 1974. In particular, the reader can consult the first Gohberg–Krein reference and the Dunford–Schwartz reference for more material on the content of this section. Our discussion of determinants is patterned after that in B. Simon, "Notes on infinite determinants of Hilbert space operators," *Adv. Math.* 24 (1977), 244–273. There are some elements in common with the treatment in J. R. Ringrose, *Compact Non-self-adjoint Operators*, Van Nostrand–Reinhold, Princeton, New Jersey, 1971.

If an operator has an eigenvector, it clearly has a nontrivial invariant subspace. The existence of compact operators with no eigenvalue (Example 1) leads to the question of whether every compact operator has a nontrivial invariant subspace. This problem was finally solved (positively) by J. von Neumann (unpublished) in the Hilbert space case and by N. Aronszajn and K. T. Smith, "Invariant subspaces of completely continuous operators," *Ann. Math.* 60 (1954), 345–350. There is a more general problem of whether every bounded operator on a Hilbert space has a nontrivial invariant subspace. This is discussed in H. Helson, *Lectures on Invariant Subspaces*, Academic Press, New York, 1964; W. B. Arveson and J. Feldman, "A note on invariant subspaces," *Michigan Math. J.* 15 (1968), 61–64; and C. Pearcy and N. Salinas, "An invariant subspace theorem," *Michigan Math. J.* 20 (1973), 21–31; and the relevant articles in the collection edited by C. Pearcy quoted above.

What we have called the Schur–Lalesco–Weyl theorem (Theorem XIII.103) has a complex history, in part, because the definition of trace class and $\mathscr{I}_p$ is so recent. The criterion for an infinite matrix to be Hilbert–Schmidt is rather simple (namely, that $\sum_{n,m} |a_{mn}|^2 < \infty$) and so this class was singled out rather early. I. Schur in "Über die charakteristischen Wurzeln einer linearen Substitution mit einer Anwendung auf die Theorie der Integralgleichung," *Math. Ann.* 66 (1909), 488–510, proved that $\sum_{n=1}^{N(A)} |\lambda_n(A)|^2 < \infty$ if A is Hilbert–Schmidt. T. Lalesco in "Une théorème sur les noyaux composés," *Bull. Soc. Sci. Acad. Roumania* 3 (1914–15), 271–272, proved that $\sum_{n=1}^{N(A)} |\lambda_n(A)| < \infty$ for a large class of operators that we would now call trace class. This was extended to the full trace class (expressed as an arbitrary product of two Hilbert–Schmidt operators!) by S. A. Gheorghiu, "Sur l'équation de Fredholm," Thèse, Paris, 1928, and E. Hille and J. D. Tamarkin, "On the characteristic values of linear integral equations," *Acta Math.* 57 (1931), 1–76. H. Weyl, in "Inequalities between the two kinds of eigenvalues of a linear transformation," *Proc. Nat. Acad. Sci. U.S.A.* 35 (1949), 408–411, proved the general relation that

$$\sum_{n=1}^{N(A)} \varphi(|\lambda_n(A)|) \leq \sum_{n=1}^{\infty} \varphi(\mu_n(A))$$

for any positive function φ with $\varphi(e^t)$ convex on $(-\infty, \infty)$ with $\varphi(0) = 0$. Weyl based his proof on general properties of convex functions and the inequality (Problem 154)

$$|\lambda_1(A) \cdots \lambda_n(A)| \leq \mu_1(A) \cdots \mu_n(A)$$

Our proof is taken from the Simon paper quoted above. Extensions of Weyl's result have been obtained by A. Ostrowski, "Sur quelques applications des fonctions convexes et concaves au sens de I. Schur," *J. Math. Pure Appl.* **9** (1952), 253–292; see also the first Gohberg and Krein book.

Using the inequality above, one can prove that

$$\mathrm{Tr}(\varphi(e^{A+B})) \leq \mathrm{Tr}(\varphi(e^{A/2}e^{B}e^{A/2}))$$

for any φ with $t \to \varphi(e^t)$ convex. This is a result of C. Thompson, "Inequalities and partial order on matrix spaces," *Indiana Math. J.* **21** (1971), 469–480. Our proof of the corollary to Theorem XIII.103, which is similar to one of Thompson's, was suggested to us by P. Deift. The basic bound $\|C^{1/2}DC^{1/2}\|_r \leq \|CD\|_r$ can also be proven using complex interpolation (Problem 168). For a discussion of the history of the Golden–Thompson inequality, see the notes to Section X.9.

Determinants of certain operators on infinite-dimensional spaces were introduced by I. Fredholm, "Sur une classe d'equations fonctionelles," *Acta Math.* **27** (1903), 365–390. He also introduced the function $D_\mu(A)$ in these cases in terms of the expansion of Problem 153. Fredholm dealt with operators A of the form $(Af)(x) = \int_a^b K(x, y)f(y)\,dy$ and wrote explicit formulas for $\mathrm{Tr}(\bigwedge^k(A))$ rather than using abstract multiltilinear algebra. For example

$$\mathrm{Tr}(\bigwedge^k(A)) = \frac{1}{n!}\int_a^b \cdots \int_a^b K\begin{pmatrix} x_1 & \cdots & x_n \\ x_1 & \cdots & x_n \end{pmatrix} dx_1 \cdots dx_n$$

where

$$K\begin{pmatrix} x_1 & \cdots & x_n \\ y_1 & \cdots & y_n \end{pmatrix} = \det(K(x_i, y_j))_{1 \leq i, j \leq n}$$

Fredholm's work had profound effects in the history of functional analysis leading to the abstraction of the notion of Hilbert space and to the development of the theory of compact operators. Two books describing "classical" Fredholm theory are F. Smithies, *Integral Equations*, Cambridge Univ. Press, London and New York, 1965 and W. Lovitt, *Linear Integral Equations*, Dover, New York, 1924.

Lidskii's theorem appeared in V. R. Lidskii, "Non-self-adjoint operators with a trace," *Dokl. Akad. Nauk SSSR* **125** (1959), 485–487. Our proof follows Simon's paper.

The Plemelj–Smithies formulas are due to J. Plemelj, "Zur Theorie der Fredholmschen Funktionalgleichung," *Monat. Math. Phys.* **15** (1909), 93–128; and F. Smithies, "The Fredholm theory of integral equations," *Duke Math. J.* **8** (1941), 107–130.

The theory of regularized determinants (Problem 155) for $\mathscr{I}_p$ operators is a theory with contributions made by D. Hilbert, "Grundzüge einer allgemeinen Theorie der linearen Integralgleichungen, Erste Miteilung," *Nacht. Akad. Wiss. Göttingen Math. Phys. Kl. II* (1904), 49–91; H. Poincaré, "Rémarques diverse sur l'équation de Fredholm," *Acta Math.* **33** (1910), 57–86; the papers of Plemelj and Smithies quoted above; F. Carleman, "Zur Theorie der linearen Integralgleichung," *Math. Zeit.* **9** (1921), 196–217; the paper of Hille and Tamarkin quoted in our discussion of the Schur–Lalesco–Weyl theorem; the first book of Gohberg and Krein; the book of Dunford and Schwartz; and that of H. J. Brascamp, "The Fredholm theory of integral equations for special types of compact operators on a separable Hilbert space," *Compositio Math.* **21** (1969), 59–80. This theory has turned out to be useful in studying renormalization theory in the Yukawa field theory in two space-time dimensions: See E. Seiler, "Schwinger functions for the Yukawa models in two dimensions with space-time cutoffs," *Comm.*

Math. Phys. **42** (1975), 163–182. Our treatment of $\det_n$ in Problem 155 uses some of Seiler's ideas. Theorem XIII.104, which appears in Simon's paper, is an abstraction of an argument from E. Seiler and B. Simon, "On finite mass renormalizations in the two-dimensional Yukawa model," *J. Mathematical Phys.* **16** (1975), 2289–2293.

Fredholm theory has been extended to Banach spaces by A. F. Ruston, "On the Fredholm theory of integral operators belonging to the trace class of a general Banach space," *Proc. London Math. Soc.* **53** (1951), 109–124 and "Direct products of Banach spaces and linear functional equations," *Proc. London Math. Soc.* **1** (1953), 327–384; T. Lezinski, "The Fredholm theory of linear equations in Banach spaces," *Studia Math.* **13** (1953), 244–276; and A. Grothendieck, "La Théorie de Fredholm," *Bull. Soc. Math. France* **84** (1956), 319–384. An analogue of the trace class (called nuclear operators) was developed on an arbitrary Banach space by A. Grothendieck, "*Produits tensoriel topologique et espaces nucleaires*," *Mem. Amer. Math. Soc.* **16** (1955). Grothendieck constructed an example of a nuclear operator on $L^\infty(0, 1)$ with $\sum |\lambda_n(A)|^p = \infty$ for any $p < 2$ so the Schur–Lalesco–Weyl theorem in the form $\sum |\lambda_n(A)| \leq \|A\|_1$ fails on general Banach spaces. Indeed, W. Johnson, B. Maury, H. Konig, and J. R. Retherford (in preparation) have shown that if X is a Banach space for which $\sum |\lambda_n(A)| < \infty$ for every nuclear operator, then X is topologically isomorphic to a Hilbert space! Weakened versions of the Schur–Lalesco–Weyl inequality and Lidskii's theorem on a general Banach space are discussed in the Grothendieck memoir, the paper of Johnson *et al.*, and A. S. Marcus and V. I. Macaev, "Analogs of Weyl inequalities and the trace theorem in a Banach space," *Soviet Math. Dokl.* (1972), 299–312.

Completeness theorems for the generalized eigenfunctions of accretive operators go back to M. V. Keldys, "On the characteristic values and characteristic functions of certain classes of non-self-adjoint equations," *Dokl. Akad. Nauk SSSR* **77** (1951), 11–14. Further results of Keldys, Keldys and Lidskii, and Krein and Gohberg are discussed in detail in Chapter V of the first quoted Gohberg and Krein book. Our discussion is patterned in part on that in Dunford and Schwartz.

The discussion in Example 5 follows that in B. Simon, "The bound state of weakly coupled Schrödinger operators in one and two dimensions," *Ann. Phys.* **97** (1976), 279–288. The result that $-d^2/dx^2 + \lambda V$ has a bound state for all small λ if and only if $\int V(x)\,dx \leq 0$ is proven there for all V with $\int (|x|^2 + 1)|V(x)|\,dx < \infty$. The analyticity result of Theorem XIII.110 does not require that V have compact support but only that $\int e^{a|x|}|V(x)|\,dx < \infty$ for some $a > 0$. In two dimensions, $-\Delta + \lambda V$ has a bound state for all small λ if and only if $\int V(x)\,dx \leq 0$ so long as

$$\int |V(x)|^{1+\varepsilon}\,dx < \infty \qquad \text{for some} \quad \varepsilon > 0$$

and

$$\int |V(x)|(1 + |x|^2)^{\varepsilon}\,dx < \infty \qquad \text{for some} \quad \varepsilon > 0$$

But the eigenvalue $E(\lambda)$ is *not* analytic at $\lambda = 0$ in the two-dimensional case. In fact, $|E(\lambda)| \leq \exp(-1/a\lambda)$ for suitable $a > 0$. All these results require the use of the modified determinant, $\det_2$, for $\mathscr{I}_2$ (see Problem 155). These questions are further discussed in R. Blankenbecker, M. L. Goldberger, and B. Simon, "The bound states of weakly coupled long-range one-dimensional quantum Hamiltonians," *Ann. Physics* **108** (1977), 69–78, and K. Klaus, *Ann. Physics* (to appear).

Finally, we remark that the Jost function discussed in Section XI.8 is a Fredholm determinant. The s-wave Lipmann–Schwinger equation reads

$$\psi(\cdot, k) = \psi_0(\cdot, k) - (A_k\psi)(\cdot, k) \tag{207}$$

where A_k is the integral operator with kernel

$$k^{-i}\exp[ik(\max\{x, y\})]\sin[k(\min\{x, y\})]V(y)$$

It can be shown that $\eta(k) = \det(1 + A_{-k})$, and that the factorization $S(k) = \eta(k)/\eta(-k)$ is connected with the meromorphic solution of (207).

PROBLEMS

†*1.* Prove that $\mu_n(A) \leq \mu_n(B)$ for any n if $A \leq B$ (defined in Section XIII.2).

2. Use the min–max principle to prove that

$$|\mu_k(A) - \mu_k(B)| \leq \|A - B\|$$

for bounded self-adjoint operators, where μ_k is given by Theorem XIII.1.

†*3.* Prove Theorem XIII.4.

†*4.* (a) Let $p = i\,d/dx$ on $L^2(\mathbb{R})$. Prove that

$$p^2 + x^2 + \beta x^4 \leq C_1(p^2 + x^2)^2 \leq C_2(p^2 + x^2 + \beta x^4)^2$$

for any fixed $\beta > 0$.

(b) Conclude that

$$\lim_{N\to\infty}\left(\sum_{i=1}^{N} a_i^{(n)}\varphi_i\,,\, H\left(\sum_{i=1}^{N} a_i^{(n)}\varphi_i\right)\right) = \mu_n(H)$$

if $H = p^2 + x^2 + \beta x^4$, where $\{\varphi_i\}_{i=1}^{N}$ are the eigenfunctions of $p^2 + x^2$ and $\sum a_i^{(n)}\varphi_i$ is the expansion of the nth eigenfunction of H in terms of the φ_i.

5. Let $H = p^2 + x^2 + \beta x^{2m}$. Prove the applicability of Theorem XIII.4 using the eigenfunctions of $p^2 + x^2$ as trial functions.

6. Using φ_1 and φ_3, find an upper bound on the ground state energy of $p^2 + x^2 + 0.2x^4$. Using Temple's inequality find a lower bound. Compare with the "exact" result and perturbation theory computations in Section XII.3.

7. Using a trial vector of the form $\psi(\mathbf{r}) = c\exp(-\alpha r^2)$ and varying α, compute an upper bound for the ground state of $-\Delta - r^{-1}$ and compare with the exact answer.

8. Write a computer program to compute the lowest eigenvalue of $p^2 + x^2 + x^4$ to six-place accuracy.

9. Let $\lambda_n(c)$ denote the nth eigenvalue of $-d^2/dx^2 + x^2 + cx^4$ for $c \geq 0$. Find a constant $c_0 > 0$ so that $\lambda_2(c) - \lambda_1(c) \geq c_0$ for all c. (Hint: Compare the $\lambda_n(c)$ to the eigenvalues of $-d^2/dx^2 + x^2$ and $-d^2/dx^2 + cx^4$ and use the min–max principle.)

10. Find and prove an analog of Theorem XIII.4 for excited states.

11. (Rayleigh's theorem) Let $\mu_1, \ldots, \mu_n$ be the eigenvalues of an $n \times n$ Hermitian matrix and let $\lambda_1, \ldots, \lambda_{n-1}$ be the eigenvalues of its restriction to an $(n-1)$-dimensional subspace. Prove that $\mu_1 \leq \lambda_1 \leq \mu_2 \leq \lambda_2 \leq \cdots \leq \mu_{n-1} \leq \lambda_{n-1} \leq \mu_n$.

12. Suppose that V is a regular perturbation of H_0 and that H_0 has a discrete, nondegenerate ground state. Let $E(\lambda)$ be the ground state energy for $H_0 + \lambda V$ and $\psi(\lambda)$ the normalized ground state eigenvector. Suppose that $\varphi(\lambda)$ is given so that $\|\varphi(\lambda)\|^{-1}\varphi(\lambda) - \psi(\lambda) = O(\lambda^{n+1})$ in H_0-graph norm and $\|\varphi(\lambda)\| = 1 + O(\lambda)$ (for example, $\varphi(\lambda)$ could be the first n terms of an unnormalized Rayleigh–Schrödinger expansion).

(a) Prove that $(H(\lambda) - E(\lambda))\varphi(\lambda) = O(\lambda^{n+1})$.

(b) Prove that

$$(\varphi(\lambda), H(\lambda)^2\varphi(\lambda))\|\varphi(\lambda)\|^2 - (\varphi(\lambda), H(\lambda)\varphi(\lambda))^2 = O(\lambda^{2n+2})$$

(c) Using Temple's inequality, prove that $E(\lambda) - \|\varphi(\lambda)\|^{-2}(\varphi(\lambda), H(\lambda)\varphi(\lambda)) = O(\lambda^{2n+2})$.

Reference: E. Harrel, II, Princeton Univ. Thesis, Princeton, New Jersey, 1976.

13. (a) Suppose that P is a projection and that $V > 0$ is a positive operator and H_0 is self-adjoint. Prove that as quadratic forms $H_0 + V \geq H_0 + V^{1/2}PV^{1/2}$.

(b) Let A be self-adjoint with Ker $A = 0$ and let Q be a finite-dimensional projection so that Ran $Q \subset D(V^{-1/2}A)$. Let $(QAV^{-1}AQ)^{-1}$ denote the inverse of the operator $QAV^{-1}AQ$ on Ran Q. Prove that

$$P = V^{-1/2}AQ(QAV^{-1}AQ)^{-1}QAV^{-1/2}$$

is a projection and conclude that

$$H_0 + V \geq H_0 + AQ(QAV^{-1}AQ)^{-1}QA$$

(c) Prove that if ψ_0 is an eigenvector of H_0, then

$$H_0 + (\psi_0, V^{-1}\psi_0)^{-1}(\psi_0, \cdot)\psi_0 \leq H_0 + V$$

(Hint: Use $A = 1$, $Q = (\psi_0, \cdot)\psi_0$.)

Reference for Part (c): W. Thirring, *Vorlesungen Über Mathematische Physik, T7: Quantenmechanik*, Universität Wien Lecture Notes, Section 2.9.

14. (a) Suppose that $\sigma(H) \cap (a, b) = \varnothing$ for some self-adjoint operator H. Let φ be in $D(H)$ with $\|\varphi\| = 1$. Prove that

$$\left(\varphi, \left[H - \left(\frac{a+b}{2}\right)\right]^2\varphi\right) \geq \left(\frac{a-b}{2}\right)^2$$

(b) Rewrite (a) in terms of $\gamma = (\varphi, H\varphi)$ and $\eta = (\varphi, H^2\varphi) - (\varphi, H\varphi)^2$ to read $\eta \geq (\gamma - a)(b - \gamma)$.

(c) Conclude that, if $\varphi \in D(H)$ with

$$\eta < (\gamma - a)(b - \gamma)$$

then $\sigma(H) \cap (a, b) \neq \varnothing$.

15. (generalized Temple's inequality) Suppose that $\sigma(H) \cap (a, b)$ consists of a single point λ. Let φ be a trial vector so that $\varphi \in D(H)$ and

$$\eta < (\gamma - a)(b - \gamma) \tag{208}$$

where $\gamma = (\varphi, H\varphi)$; $\eta = (\varphi, H^2\varphi) - \gamma^2$.

(a) Prove that $\gamma \in (a, b)$.

(b) Let $a' = \gamma - (b - \alpha)^{-1}\eta$ and $b' = \gamma + (\gamma - a)^{-1}\eta$. Prove that $a < a' < b' < b$.

(c) Let $a < a'' < a'$. Prove that $\eta < (\gamma - a'')(b - \gamma)$ and conclude that $\sigma(H) \cap (a'', b) \neq \varnothing$ (use Problem 14).

(d) Prove the generalized Temple's inequality, i.e., that under the hypothesis (208) we can conclude

$$\gamma - (b - \gamma)^{-1}\eta < \lambda < \gamma + (\gamma - a)^{-1}\eta$$

Remark See the Notes to Section XIII.2 for references to this problem.

†*16.* (a) Prove that

$$H_\ell = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r)$$

is essentially self-adjoint on $\{u \mid u \in C_0^\infty(0, \infty)\}$ if $\ell \neq 0$ and $V \in C_0^\infty(0, \infty)$.

(b) Prove that $H_0 = -d^2/dr^2 + V(r)$ is essentially self-adjoint on $\{u \mid u \in C_0^\infty[0, \infty), u(0) = 0\}$.

†*17.* Let $\varphi \in C_0^\infty(\mathbb{R})$ have isolated zeros within its support. Let $H_0 = -d^2/dx^2$ on the usual domain. Prove that $|\varphi| \in Q(H_0)$.

18. (Calogero's bound) Let $V \in C_0^\infty[0, \infty)$ be negative. Let u be the solution of $u'' = Vu$; $u(0) = 0$; $u'(0) = 1$. Define $v(r)$ by $\tan v(r) = |V(r)|^{1/2}u(r)/u'(r)$.

(a) Prove that v obeys the equations

$$v'(r) = |V(r)|^{1/2} - \tfrac{1}{2}(V'(r)/|V(r)|)\cos^2 v \tan v$$

$$v(0) = 0$$

(b) Conclude that if V is monotone, $N(V) \leq (2/\pi)\int_0^\infty |V(r)|^{1/2}\,dr$.

19. (Bargmann's bound) Let u solve $u'' = [\ell(\ell+1)r^{-2} + V(r)]u$; $u(0) = 0$.

(a) Define $a_\ell(r)$ by

$$u'(r)[r^{\ell+1} + a_\ell(r)r^{-\ell}] = u(r)[(\ell+1)r^\ell - \ell a_\ell(r)r^{-\ell-1}]$$

Prove that

$$a_\ell'(r) = -(2\ell+1)^{-1}V(r)r^{-2\ell}[r^{2\ell+1} + a_\ell(r)]^2$$

(b) Let $b_\ell(r) = a_\ell(r)/r^{2\ell+1}$. Prove that $b_\ell(0) = 0$ and that

$$b_\ell'(r) \leq (2\ell+1)^{-1}r|V(r)|[b_\ell(r) + 1]^2$$

in the region where b is positive.

(c) Prove Bargmann's bound (Theorem XIII.9a) for general ℓ.

20. (a) Use Neumann bracketing (Section 15) to prove that if V is bounded with compact support, then $-\Delta + \lambda V$ has at most one negative eigenvalue for λ small.

(b) Use Neumann bracketing to prove that if V is a bounded function on $\mathbb{R}^n$ with compact support, then $-\Delta + V$ has only finitely many negative eigenvalues.

21. Find a potential V on $L^2(\mathbb{R})$ having compact support, with V negative on some open set, so that $-d^2/dx^2 + V$ has no negative eigenvalues.

**22.* Let V be a function on $\mathbb{R}$ with $\int_{-\infty}^{\infty} r|V(r)|\,dr < \infty$. Prove that $-d^2/dx^2 + V$ has at most $1 + \int_{-\infty}^{\infty} r|V(r)|\,dr$ bound states. (Hint: Use Bargmann's bound and Dirichlet boundary conditions.)

23. (a) Fix ℓ. Let V be a central potential with $n_\ell(V) = n$. Show that $V = V_1 + \cdots + V_n$ where the V_i have disjoint support and $n_\ell(V_i) \geq 1$. (Hint: Use the zeros of $u_\ell(r; E = 0)$.)
(b) Suppose that it is known that $n_\ell(V) = 0$ if

$$\int_0^\infty f(x)g(V(x))\,dx < 1$$

for fixed f, g real and positive. Prove that

$$n_\ell(V) \leq \int_0^\infty f(x)g(V(x))\,dx$$

Reference: The Grosse, Martin, Glaser, and Thirring paper quoted in the Notes to Section 3.

24. (a) Let $n \geq 3$. Let $V \leq 0$ almost everywhere. Prove that $N(V) = 0$ if and only if $|V|^{1/2}(-\Delta)^{-1}|V|^{1/2}$ has norm less than 1.
(b) Let $n \geq 3$ and let $0 \leq \alpha \leq 1$. Show that there exists a constant $C_{\alpha,n}$ so that if $\|r^\alpha |V|^{1/2}\|_{n/1-\alpha} \leq C_{\alpha,n}$, then $N(V) = 0$. (Hint: Look at the proof of Strichartz theorem, Theorem X.21.)
(c) Let $n_0(V)$ be the number of bound states of angular momentum zero in $\mathbb{R}^3$. Prove that for $\frac{1}{2} \leq \alpha < \infty$ there exists a constant $\tilde{C}_{\alpha,1}$ so that $n_0(V) = 0$ if

$$\int r^{\alpha/1-\alpha}|V(r)|^{1/(2-2\alpha)}\,dr \leq \tilde{C}_{\alpha,1}$$

(d) Prove the GGMT bound except for the precise constant.
Reference for (a)–(c): The paper of Glaser *et al.* and the review article of Simon quoted in the Notes of Section 3.

†25. (a) Let A be a positive self-adjoint operator and let B be a form-bounded perturbation of A with relative bound 0. Suppose that $[0, \infty) \subset \sigma(A + \lambda B)$ for all $\lambda \in \mathbb{R}$. Prove that $\mu_n(A + \lambda B)$ is a monotone decreasing continuous function of $\lambda \in (0, \infty)$ by using the min–max principle.
(b) Suppose $\sigma_{\text{ess}}(A + \lambda B) = [0, \infty)$ for all $\lambda \in (0, \infty)$. Prove the result of (a) by employing the perturbation theory of Chapter XII.

†26. Fill in the details in the proof of Theorem XIII.10.

27. Prove the Ghirardi–Rimini bound

$$N(V) \leq \left(\frac{1}{4\pi}\right)^2 \int \frac{V(x)V(y)}{|x-y|^2}\,d^3x\,d^3y$$

28. (a) Let $V \in R$ and let $\{P_\Omega^\lambda\}$ be the spectral projections of $-\Delta + \lambda V$. Let $\lambda > 1$. Prove that

$$\dim(\text{Ran } P^\lambda_{(-\infty,0)}) \geq \dim(\text{Ran } P^1_{(-\infty,0]})$$

(b) Conclude that

$$\dim(\text{Ran } P^1_{(-\infty,0]}) \leq (4\pi)^{-2} \int |x-y|^{-2}|V(x)|\,|V(y)|\,d^3x\,d^3y$$

†*29. Prove that for $V, W \in C_0^\infty(\mathbb{R}^n)$,

$$\int d\mu_{x,y;t} V(\omega(s)) \exp\left(-\int_0^t W(\omega(s))\, ds\right)$$

is continuous in x, y, t for $t > 0$, $x, y \in \mathbb{R}^n$ where $d\mu_{x,y;t}$ is the conditional Wiener measure. (Hint: It will help to realize all integrations over the same set of paths by mapping paths ω going from 0 to 0 in time 1, to paths ω going from x to y in time t by

$$\tilde{\omega}(s) = \omega(st^{-1}) + x + (y - x)st^{-1}$$

†30. (a) Suppose that A is a trace class operator on $L^2(\mathbb{R}^n)$ with an integral kernel $K(x, y)$ that is pointwise positive and continuous. Prove that $\mathrm{Tr}(A) = \int K(x, x)\, dx$. (Hint: Let P_n be a sequence of projections onto finite-dimensional spaces of functions piecewise constant on $\mathbb{R}^n$ so that $P_n \to I$ strongly. Write $\mathrm{Tr}(A) = \lim_{n\to\infty} \mathrm{Tr}(P_n A P_n)$ and evaluate it explicitly.)

(b) For $W \in L^1(\mathbb{R}^n)$, prove that $W^{1/2}e^{-tH_0}$ is Hilbert–Schmidt. For $W \in L^1(\mathbb{R}^n)$ and $V \geq 0$, prove that $W^{1/2}e^{-t(H_0+V)}$ is Hilbert–Schmidt.

(c) Prove (14).

31. (a) Let $N_\alpha(V)$ be the number of eigenvalues of $-\Delta + V$ on $L^2(\mathbb{R}^3)$ less than $-\alpha$. Use the Birman–Schwinger bound and Young's inequality to prove that

$$N_\alpha(V) \leq (4\pi)^{-1}(\sqrt{2\alpha})^{-1} \int \left|\min\left\{V(x) + \frac{\alpha}{2}, 0\right\}\right|^2 dx$$

(b) Let $E_1(V), \ldots, E_n(V)$ be the negative eigenvalues of $-\Delta + V$. Prove that

$$\sum_i |E_i(V)| = \int_0^\infty N_\alpha(V)\, d\alpha$$

(c) Prove the Lieb–Thirring bound

$$\sum_i |E_i(V)| \leq \frac{4}{15\pi} \int |V_-(x)|^{5/2}\, dx$$

32. Let $S_\gamma(V)$ be the sum of the numbers $|E|^\gamma$ over all negative eigenvalues of $-\Delta + V$.

(a) Prove that $S_\gamma(V) = \gamma \int_0^\infty E^{\gamma-1} N_E(V)\, dE$, if $\gamma > 0$ and $N_E(V)$ is the number of eigenvalues less than $-E$.

(b) Prove that for $V \in C_0^\infty$ and $W = -V_-$,

$$S_\gamma(V) \leq \gamma\Gamma(\gamma)(m+1) \int_0^\infty t^{-\gamma} \mathrm{Tr}\left[\sum_{j=0}^m \binom{m}{j} (-1)^j e^{-(H_0 + jW)t}\right] dt$$

for any m. $\Gamma(\cdot)$ is the Euler gamma function $\Gamma(\alpha) = \int_0^\infty u^{\alpha-1}e^{-u}\, du$.

(c) Prove that if V is a function on $\mathbb{R}^n$ and γ is any number with $\gamma \geq 0$ and $\gamma + \frac{1}{2}n > 1$, then

$$S_\gamma(V) \leq C_{n,\gamma} \int |V_-(x)|^{n/2+\gamma}\, d^n x$$

33. (a) Prove that for $n \geq 3$,

$$N_E(V) \leq C_n \int |(E + V)_-(x)|^{n/2}\, d^n x$$

by using the Cwikel–Lieb–Rosenbljum bound.

(b) Prove that for $V \in C_0^\infty$,

$$\gamma \int_0^\infty dE \int |(E + V)_-(x)|^{n/2} E^{\gamma - 1}\, dx = d_\gamma \int |V_-(x)|^{n/2 + \gamma}\, dx$$

where $d_\gamma = \gamma \int_0^1 (1 - E)^{n/2} E^{\gamma - 1}\, dE$.

(c) Provide an alternative proof of the bound of Problem 32c.

Remark The bounds of Problems 31, 32c, and 33c for $\gamma > 0$ are due to E. Lieb and W. Thirring, "Inequalities for the moments of the eigenvalues of the Schrödinger equation and their relation to Sobolev inequalities," in *Studies in Mathematical Physics: Essays in Honor of Valentine Bargmann* (E. Lieb, B. Simon, and A. S. Wightman, eds.), Princeton Univ. Press, Princeton, New Jersey, 1976. Their method of proof is illustrated in Problem 31.

34. (a) Let C be compact and let $A(z) = z^{-1}C$. Show that $(1 - A(z))^{-1}$ exists if and only if z is not an eigenvalue of C. Prove that the conclusion of Theorem XIII.13 may fail if $A(z)$ has compact residues instead of finite rank residues.

(b) Let $A(z) = \sum_{n=1}^\infty z^{-n} n P_n$ where $\{P_n\}$ is a family of rank-one projections with $P_n P_m = 0$ if $n \neq m$. Prove that the conclusions of Theorem XIII.13 may fail if $A(z)$ has essential singularities.

†*35.* Prove that $\sigma_{ess}(A)$ is a closed subset of $\mathbb{C}$ for any closed operator.

†*36.* Prove (b) of the strong spectral mapping theorem (Lemma 2 in Section 4).

37. Let A and B be positive self-adjoint operators such that $(A + 1)^{-n} - (B + 1)^{-n}$ is compact for some positive integer n. Prove that $\sigma_{ess}(A) = \sigma_{ess}(B)$.

38. (a) Let A and C be closed operators with $D(C) \supset D(A)$. Prove that $C(A - z)^{-1}$ is compact for some $z \in \rho(A)$ if and only if it is compact for all $z \in \rho(A)$.

(b) Prove that $C(A - z)^{-1}$ is compact if and only if C is a compact map from $\langle D(A), \|\cdot\|_A \rangle$ to $\langle \mathscr{H}, \|\cdot\| \rangle$ where $\|\psi\|_A^2 = \|\psi\|^2 + \|A\psi\|^2$.

39. Let A be self-adjoint and positive. A bounded form perturbation C of A is called **relatively form compact** if and only if C is compact from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$. Prove that if C is relatively form compact, then C has relative form bound zero and $\sigma_{ess}(A) = \sigma_{ess}(A + C)$.

40. Find a symmetric operator H with self-adjoint extensions A and B so that $\sigma_{ess}(A) \neq \sigma_{ess}(B)$. (Hint: Let h be a symmetric operator with deficiency indices (1, 1) and let a and b be suitable self-adjoint extensions. Take $H = h \otimes I$, $A = a \otimes I$, and $B = b \otimes I$ where I is the identity on ℓ_2.)

41. Let $V \in L^q(\mathbb{R}^n) + L_\varepsilon^\infty(\mathbb{R}^n)$ with $q \geq \max\{n/2, 2\}$ if $n \neq 4$ and $q > 2$ if $n = 4$. Prove that V is a relatively compact perturbation of $-\Delta$ so that $\sigma_{ess}(-\Delta + V) = [0, \infty)$.

†*42.* Using Theorem XIII.17, prove that

$$\inf\{\Sigma_D | \#(D) = m + 1\} \geq \inf\{\Sigma_D | \#(D) = m\}$$

and conclude that

$$\inf\{\Sigma_D | \#(D) = 2\} = \inf\{\Sigma_D | \#(D) \geq 2\}$$

43. (a) Suppose that $U(t)$ is a one-parameter unitary group whose infinitesimal generator has purely absolutely continuous spectrum. Let A be compact operator satisfying $AU(t) = U(t)A$. Prove that $A = 0$ (Hint: Prove that w-$\lim_{t\to\infty} U(t) = 0$.)

†(b) Prove that the operators associated with disconnected diagrams (according to either of the rules in Section 5) are not compact. We emphasize that the center of mass motion has been removed.

†*44.* (a) Given $V \in R$, show that there exist $V^{(n)} \in C_0^\infty$ so that $\|V^{(n)} - V\|_R \to 0$ as $n \to \infty$.

(b) Given $V \in R + (L^\infty)_\varepsilon$, show that there exist $V^{(n)} \in C_0^\infty$ so that $\|(H_0 + 1)^{-1/2}(V_n - V) \times (H_0 + 1)^{-1/2}\| \to 0$ as $n \to \infty$.

(c) Given $V_{ij} \in R + (L^\infty)_\varepsilon$, $1 \le i < j < N$, show that there exist $V_{ij}^{(n)} \in C_0^\infty$ so that $H^{(n)} = H_0 + \sum_{i<j} V_{ij}^{(n)}$ converges in norm resolvent sense to $H = H_0 + \sum_{i<j} V_{ij}$.

45. (a) Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)_\varepsilon$ and $\psi \in D(\Delta)$. Define $\psi_a(x) = \psi(x - a)$ for $a \in \mathbb{R}^3$. Prove that $\lim_{a\to\infty} \|V\psi_a\| = 0$.

(b) Prove that $\lim_{a\to\infty} \|(-\Delta + V - \lambda)\psi_a\| = \|(-\Delta - \lambda)\psi\|$ and conclude that $[0, \infty) \subset \sigma(-\Delta + V)$.

(c) Let H be the Hamiltonian $H_0 + \sum_{i<j} V_{ij}$ with $V_{ij} \in L^2 + (L^\infty)_\varepsilon$. Prove that $[\Sigma, \infty) \subset \sigma(H)$ without using wave operators.

Remark This method was used by Hunziker in the paper cited in the Notes to Section 5.

46. Let $\tilde{H}_0^{(N)} = \sum_{i=1}^N (2m)^{-1}\Delta_i$ and $H^{(N)} = H_0^{(N)} + \sum_{i<j} V(r_i - r_j)$ (all V_{ij} are the same function). Suppose that $V \in R + (L^\infty)_\varepsilon$. Let $\mathscr{H}_{\text{Fermi}}^{(N)}$ be the subspace of $L^2(\mathbb{R}^{3N-3})$ of functions odd under the coordinate change induced by the interchange of any two particles. Let $H_F^{(N)} = H^{(N)} \restriction \mathscr{H}_{\text{Fermi}}^{(N)}$. Prove that

$$\sigma_{\text{ess}}(H_F^{(N)}) = [\Sigma, \infty)$$

where $\Sigma = \inf \sigma(H_F^{(N-1)})$.

Remark 1 To prove the analogue of Lemma 1 in our proof of the HVZ theorem, it is easier to use Hunziker's method (Problem 45) rather than wave operators.

Remark 2 For extensions to other permutation symmetries and symmetry groups, see the papers of Simon, Balslev, and Zhislin and Sigalov cited in the Notes to Section 5.

47. (a) Suppose the basic smoothness estimate (31) holds for a dense set of φ. Prove that for any φ, $R(\lambda \pm i\varepsilon)\varphi \in D(A)$ a.e. in λ (ε fixed, $\varepsilon \neq 0$) and that (31) holds.

(b) Suppose that for a fixed $\varepsilon > 0$, $\int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2 \, d\lambda < \infty$ for each $\varphi \in \mathscr{H}$. Prove that

$$\int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2 \, d\lambda \le C\|\varphi\|^2$$

for some C and all φ. (Hint: Apply the closed graph theorem to the map $\varphi \mapsto AR(\lambda + i\varepsilon)\varphi$ of $\mathscr{H}$ into $L^2(\mathbb{R}, d\lambda; \mathscr{H})$.)

(c) Suppose that $\sup_{\varepsilon>0} \int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2 \, d\lambda < \infty$ for each φ. Prove that A is H-smooth. (Hint: Use (b) and the uniform boundedness principle.)

48. Let f be a bounded Borel function on $\mathbb{R}$ and suppose $f(H)$ is H-smooth for some self-adjoint operator H. Prove that $f(H) = 0$.

49. (a) Let H be self-adjoint and let A be H-smooth. Prove that A is $|H|^\alpha$-bounded for any $\alpha > \frac{1}{2}$. (Hint: Use form (3) of Theorem XIII.25 to prove that $(H^2 + 1)^{-\alpha/2}A^*$ is bounded.)

(b) Let $H = -i\, d/dx$ on $L^2(\mathbb{R})$. Prove that there exist $\varphi \in Q(H)$ that are not bounded.
(c) Find an H-smooth operator A so that A is not $|H|^{1/2}$-bounded. (Hint: Use Example 1.)

50. Let H be multiplication by x on $L^2([\alpha, \beta], dx)$ with $\alpha, \beta \in \mathbb{R}$. Suppose that A is bounded and A^*A has integral kernel K. Prove that $\|A\|_H^2 \equiv \|K\|_\infty$.

**51.* Let H be multiplication by x on $L^2([\alpha, \beta], dx)$ with $\alpha, \beta \in \mathbb{R}$. Suppose that A is bounded and H-smooth. Prove that A^*A has the form (37). (Hint: First show that A^*x is in L^∞ for every x with $\|A^*x\|_\infty \leq C\|x\|_2$ and then use the Dunford–Pettis theorem (Problem 33 in Chapter V) to find a bounded measurable function F from $[\alpha, \beta]$ to $\mathscr{H}$, so that $(A^*x)(\lambda) = (F(\lambda), x)$.
Reference for Problem 51: Kato's *Studia Math.* paper (see the Notes to Section 7).

52. Let A and B be self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. Suppose C is A-smooth and D is a bounded operator on $\mathscr{H}_2$. Prove that $C \otimes D$ is $A \otimes I + I \otimes B$-smooth.

53. Under the hypotheses of Theorem XIII.26, prove that for any $\lambda \in \mathbb{C}$ with $|\lambda| \leq 1$, $H_0 + \lambda \sum_{i=1}^n C_i$ is a strictly m-accretive form on $Q(H_0)$, and that the associated operator H has $\sigma(H) \subset \sigma(H_0)$ and obeys $\sup \| |C_i|^{1/2}(H - z)^{-1} |C_j|^{1/2} \| < \infty$ for all i, j (continued in the next problem).

**54.* (continued from Problem 53) Let $R(\mu)$ be the resolvent of H_0 and $R(\mu; \lambda)$ the resolvent of $H(\lambda) = H_0 + \lambda \sum_{i=1}^n C_i$. Define $W^\pm(\lambda)$ by

$$(\varphi, W_\pm(\lambda)\psi) = (\varphi, \psi) \mp \frac{\lambda}{2\pi i} \sum_{i=1}^{n} \int_{-\infty}^{\infty} (C_i^{1/2} R(\mu \pm i0)\varphi,\ |C_i|^{1/2} R(\mu \mp i0, \lambda)\psi)\, d\mu$$

Prove that
(a) $W_\pm(\lambda)$ are analytic in the region $|\lambda| \leq 1$.
(b) $W_\pm(\lambda)$ are invertible and $H(\lambda) = W_\pm(\lambda) H_0 W_\pm(\lambda)^{-1}$.
(c) If λ is real, $W^\pm(\lambda) = \Omega^\pm(\lambda)$.

55. Let A and H_0 be self-adjoint operators with $\mathrm{Ker}(A) = \{0\}$. Prove that, for any positive integers $n \neq m$, at most one of A^n and A^{-m} is H_0 smooth.

56. Let $V \in R$, the Rollnik class, with $\|V\|_R < 4\pi$. Prove that the wave operators provide unitary equivalences of $-\Delta$ and $-\Delta + V$ and in particular that scattering is complete.

57. (a) Let $H_n = H_0 + A_n^* B_n$ where B_n is H_0-smooth and A_n is H_n-smooth. Suppose that $\sup_n \|A_n\|_{H_n} < \infty$ and $\lim_{n\to\infty} \|B_n\|_{H_0} = 0$. Prove that $\Omega_n^\pm \equiv \text{s-lim}_{t \to \mp\infty} e^{itH_n} e^{-itH_0}$ converges to 1 *in norm*. In particular verify the norm continuity of $\Omega^\pm(\lambda) = \text{s-lim}_{t\to\mp\infty} e^{it(H_0 + \lambda C)} e^{-itH_0}$ for $\lambda \in (-1, 1)$, in the context of Theorem XIII.26.
(b) Let $V_n \to V$ in Rollnik norm. Prove that the corresponding S matrices converge strongly. (Hint: Write $V_n = W_n + Y_n$, $V = W + Y$, so that $Y_n \to Y$ in $L^1 \cap R$, $W_n \to W$ in R, and $\sup_n \|W_n\|_R < 4\pi$.)

58. (a) Let H_0 be the operator on $L^2[0, \infty)$ that is the closure of $-d^2/dx^2$ on $\{u \in C_0^\infty[0, \infty) \mid u(0) = 0\}$. Let $E \notin \sigma(H_0)$ and let

$$K_E(x, y) = E^{-1/2} \sin[\sqrt{E} \min\{x, y\}] \exp[i\sqrt{E} \max\{x, y\}]$$

where $\sqrt{E}$ is the square root with $\operatorname{Im}\sqrt{E} > 0$. Prove that

$$[(H_0 - E)^{-1}\varphi](y) = \int_0^\infty K_E(x, y)\varphi(y)\, dy$$

(b) $|K_E(x, y)| \leq \sqrt{xy}$.
(c) Let V be a measurable function on $[0, \infty)$ with $\int_0^\infty x|V(x)|\, dx < \infty$. Then,

$$\sup_{E \notin \mathbb{R}} \| |V|^{1/2}(H_0 - E)^{-1}|V|^{1/2}\| < \infty$$

(d) If $\int_0^\infty x|V(x)|\, dx < 1$, then H_0 and $H_0 + V$ are unitarily equivalent and the wave operators are unitary equivalences.

59. Let A and H be bounded self-adjoint operators and let $R(\mu) = (H - \mu)^{-1}$. Prove that

$$|\varepsilon|\, |(R(\lambda + i\varepsilon)\varphi, [H, A]R(\lambda + i\varepsilon)\varphi)| \leq \|A\|\, \|\varphi\|^2$$

and use this to prove that $(i[H, A])^{1/2}$ is H-smooth if $i[H, A] \geq 0$.

60. Let A and B be bounded self-adjoint operators and c a strictly positive real number. Prove that $i[A, B] \geq cI$ is impossible by:
(a) using the theory of smooth perturbations;
(b) direct computation (look at $e^{iAt}Be^{-iAt}$).

61. Extend the Kato–Putnam theorem to the case where H is unbounded and $i[H, A] > 0$ means that $i(A\varphi, H\varphi) - i(H\varphi, A\varphi) > 0$ for all $\varphi \in D(H)$, $\varphi \neq 0$.

†*62.* Suppose that $f(t)$ is a Banach-space-valued uniformly continuous function on $\mathbb{R}$. Suppose also that $\int_{-\infty}^{\infty} \|f(t)\|^p\, dt < \infty$ for some $p < \infty$. Suppose that f is strongly differentiable with a uniformly bounded derivative. Conclude that $\lim_{t\to\infty} f(t) = 0$.

†*63.* Fill in the computations in the proof of Theorem XIII.29.

†*64.* Fill in the details of the proof of Theorem XIII.32.

65. By iterating the proof of (a) in Theorem XIII.33, prove that if $H_0\varphi = \lambda\varphi - V\varphi$ with $\lambda > 0$, then $\varphi \in L^2_\delta$ for all δ.

†*66.* (a) Prove that $(-\Delta - \mu)^{-1}$ is bounded from L^2_δ to L^2_δ for any δ and any $\mu \in \mathbb{C}\backslash\mathbb{R}$. (Hint: Prove it for $\delta > 0$ inductively in $[0, 1]$, $(1, 2]$, ...)
(b) Complete the proof of Lemma 1 in Section 8.
(c) Prove that $(-\Delta + 1)^{-1}\, \partial/\partial x_i$ is a bounded map from L^2_δ to L^2_δ for any δ.

†*67.* Verify the bound (62).

68. Let $\delta > n + \frac{1}{2}$. Prove that, for any $b > a > 0$, there is a constant C so that

$$\|(-\Delta - \lambda - i0)^{-m}\varphi\|_{-\delta} \leq C\|\varphi\|_\delta$$

for all $\varphi \in \mathscr{S}(\mathbb{R}^m)$ and all $\lambda \in [a, b]$.

69. Let $\|A\|_{\delta, -\delta}$ denote the norm of A as a map of L^2_δ to $L^2_{-\delta}$. Let $\delta > \frac{1}{2}$. Prove that for any $\alpha < \min\{1, \delta - \frac{1}{2}\}$, $(H_0 - \mu - i0)^{-1}$ is Hölder continuous of order α as an $\mathscr{L}(L^2_\delta, L^2_{-\delta})$-valued function of μ, i.e., for any $\mu > 0$, there is a C and an ε so that

$$\|(H_0 - \mu' - i0)^{-1} - (H_0 - \mu - i0)^{-1}\|_{\delta, -\delta} \leq C|\mu - \mu'|^\alpha$$

if $|\mu - \mu'| < \varepsilon$.

*70. Let V be an Agmon potential. Let $a_1, \ldots, a_n$ obey $\sum_{i=1}^n \partial_j a_j = 0$ (distributional sense) with $|a_j(x)| \leq C_j(1 + |x|^2)^{-1/2-\varepsilon}$. Let

$$H = -\Delta + 2i\sum_{j=1}^n a_j \partial_j + \sum_{j=1}^n a_j^2 + V$$

Prove that $\sigma_{\text{sing}}(H) = \varnothing$ and that $\Omega^{\pm}(H, H_0)$ exist and are complete. (Hint: Develop a theory paralleling Theorem XIII.33.)

*71. Suppose $V(x) = (1 + |x|^2)^{-1/2-\varepsilon}W(x)$ where W is a form relatively compact perturbation of $-\Delta$. Prove that Theorem XIII.33 remains valid.

72. Let $A \geq 0$ be a positive self-adjoint operator and let $\mathscr{H}_{+1} \subset \mathscr{H} \subset \mathscr{H}_{-1}$ be the corresponding scale of spaces. Let $U(s)$ be a unitary group on $\mathscr{H}$ with each $U(s)$ in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{+1})$. Let $V \in \mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ and define $V(s) = U(s)VU(s)^{-1}$ for $s \in \mathbb{R}$. Prove that if $V(s)$ can be continued to an $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$-valued analytic function in a neighborhood of $s = 0$, it can be continued to an entire strip $\{s \mid |\text{Im } s| < \alpha\}$.

73. (a) Let H_0 be a positive self-adjoint operator and let V be a symmetric operator with $D(V) \supset D(H_0)$. Suppose that $V(H_0 + 1)^{-1}$ is a compact operator. Prove that $(H_0 + 1)^{-1/2}V(H_0 + 1)^{-1/2}$ is compact. (Hint: Use interpolation.)

(b) Call an operator V on $L^2(\mathbb{R}^3)$ in class C_α if and only if:

(1) V is a symmetric operator with $D(V) \supset D(H_0)$ where $H_0 = -\Delta$.

(2) $V(H_0 + 1)^{-1}$ is compact.

(3) The family of operators $\tilde{F}(\theta) = u(\theta)Vu(\theta)^{-1}(H_0 + 1)^{-1}$ defined for $\theta \in \mathbb{R}$ has an extension to an analytic operator-valued function in the strip $\{\theta \mid |\text{Im } \theta| < \alpha\}$.

Prove that $C_\alpha \subset \mathscr{F}_\alpha$.

†74. Supply the details for Example 1 in Section 10.

75. Let A be a self-adjoint operator and let $U(s) = e^{isA}$ be the generated unitary group. Let $\psi \in C^\infty(A)$ with $\sum_{n=0}^\infty t^n\|A^n\psi\|/n! < \infty$ if $|t| < \alpha$. Prove that $f(s) = e^{isA}\psi$ has an analytic continuation into the strip $\{s \mid |\text{Im } s| < \alpha\}$. Conversely, if $f(s)$ has such a continuation, prove that $\sum_{n=0}^\infty t^n\|A^n\psi\|/n! < \infty$ if $|t| < \alpha$.

†76. Provide the necessary connectedness argument needed in the proof of Theorem XIII.36 to show that if γ is a curve in B_α and $\lambda \notin \sigma_{\text{ess}}(H(\gamma(t)))$ for any t, then either λ is in both $\sigma_d(\gamma(0))$ and $\sigma_d(\gamma(1))$ or in neither.

†77. Fill in the details of the proof of Proposition 2 in Section 10.

†78. Under the hypotheses of Theorem XIII.37, prove that

$$\{\mu + e^{-2\theta}\lambda \mid \mu \in \sum(\theta), \lambda \in [0, \infty)\} \subset \sigma_{\text{ess}}(\theta)$$

by the following procedure:

(a) Suppose first that each $V_{ij} \in C_\alpha$ (see Problem 73). (Hint: See Problem 45.)

(b) Use a limiting argument if $V_{ij} \in \mathscr{F}_\alpha$.

†79. Fill in the details of the proof of Theorem XIII.37.

†80. Prove Lemma 1b of Section 11.

†81. Let $V \in M_\sigma^{(n)}$ with $\sigma > n/2$, $\sigma \geq 1$. Prove that $V << -\Delta$.

†82. Under the hypotheses of Theorem XIII.38, prove that the embeddings $C^\infty(\tilde{H}) \subset C_0$ (or C_0^1) are continuous.

83. Let $(-\Delta + V)\psi = E\psi$ in distributional sense and let V be C^∞ on Ω, an open set of $\mathbb{R}^n$. Use the ideas of the elliptic regularity theorem to prove that ψ is C^∞ on Ω.

84. Find an example to show that O'Connor's lemma does not extend to the case where $P(0)$ is an infinite-dimensional projection.

85. Under the hypotheses of O'Connor's lemma, prove that $P(\alpha)$ always extends analytically to the region $\tilde{D} \equiv \{\alpha \,|\, \text{Im } \alpha = \text{Im } \alpha_0 \text{ for some } \alpha_0 \in D\}$.

†*86.* (a) Let $0 < a < b$. Show that there exist *unit* vectors $\mathbf{e}_1, \ldots, \mathbf{e}_k$ in $\mathbb{R}^n$ so that

$$\exp(a|x|) \leq \sum_{j=1}^{k} \exp(b\mathbf{e}_j \cdot \mathbf{x})$$

for all $x \in \mathbb{R}^n$.

(b) Verify the computation of the essential spectrum of $H(\alpha)$ in the proof of Theorem XIII.40.

(c) Show that $\sigma_{ess}(H(\alpha)) \subset \{\lambda \,|\, \text{Re } \lambda \geq \Sigma - (2M)^{-1} |\text{Im } \alpha|^2\}$.

(d) Complete the proof of Theorem XIII.40.

87. Under the hypotheses of Theorem XIII.42, prove that

$$|\psi(\zeta) - \psi(\zeta')| \leq C_\varepsilon \exp[-(a - \varepsilon)\min\{r, r'\}]\,|\zeta - \zeta'|^\theta$$

so long as $\theta < \min\{1, 2 - 3/\sigma\}$. Here r (respectively, r') is the radius of gyration of the configuration ζ (respectively, ζ').

†*88.* Fill in the missing step in the proof of Theorem XIII.42.

89. (a) Let A and B be semibounded operators on a Hilbert space with $Q(A) \subset Q(B)$. Suppose that $B - A$ is strictly positive in the sense that $(\psi, (B - A)\psi) > 0$ for all $\psi \neq 0$ with $\psi \in Q(A) \cap Q(B)$. Suppose that $\mu_1(A)$ is an isolated eigenvalue of finite multiplicity. Prove that $\mu_1(A) < \mu_1(B)$. Give an example where $\mu_1(A)$ is in the essential spectrum and $\mu_1(A) = \mu_1(B)$.

(b) Prove directly that if V is central and if $-\Delta + V$ has a ground state, then it is an s-state with no nodes.

†*90.* Fill in the details in Example 2 of Section XIII.12.

91. Let H_0 be an operator that generates a positivity improving semigroup. Let $-V$ be a positivity preserving bounded operator. Prove that:

(i) $(H_0 + V + \mu)^{-1}$ is positivity improving for all sufficient large μ.

(ii) $\exp(-t(H_0 + V))$ is positivity improving for all $t > 0$.

92. Let $H_0 = -\Delta$, let V be an H_0-bounded multiplication operator with relative bound less than one, and let W be a Hilbert–Schmidt operator whose kernel is negative. Prove that $H_0 + V + W$ has a nondegenerate, strictly positive ground state if it has an eigenvalue at the bottom of its spectrum.

**93.* Find an operator that is positive, positivity preserving, and ergodic that is not positivity improving. (Hint: Look for a 3×3 matrix.)

94. Find a positive operator H_0 for which $(H_0 + \mu)^{-1}$ is positivity preserving for some but not all μ. (Hint: Look for a 3×3 matrix.)

95. Let $H(\lambda) = -d^2/dx^2 + x^2 + \lambda/x^4$ with $\lambda > 0$ and domain $C_{00}^\infty(\mathbb{R})$, the C_0^∞ functions with support away from the origin.
(a) Prove that $H(\lambda)$ is essentially self-adjoint.
(b) Prove that $H(\lambda)$ has purely discrete spectrum.
(c) Prove that the lowest eigenvalue is degenerate.
(d) Why does this not violate Theorem XIII.46?
(e) Why cannot $H(\lambda)$ converge to $-d^2/dx^2$ in strong resolvent sense as $\lambda \downarrow 0$. To what does it converge?

†96. Complete the proof of the first Beurling–Deny criterion.

97. (a) Let A be a finite matrix that is not necessarily symmetric such that $a_{ij} \leq 0$ if $i \neq j$. Prove that $\exp(-tA)$ is a matrix with positive elements for all $t > 0$. (Hint: Write $A = B + D$ with D diagonal and $b_{ij} \leq 0$ for all i, j and use the Trotter product formula.)
(b) Let A be a finite matrix that is not necessarily symmetric such that e^{-tA} is a matrix with positive elements for all $t > 0$. Prove that $a_{ij} \leq 0$ for all $i \neq j$. (Hint: Use $A = \lim_{t \downarrow 0} (1 - e^{-tA})/t$.)

98. Suppose that $H \geq 0$. Let F_n be a family of functions on $\mathbb{C}$ (respectively $\mathbb{R}$) with $|F_n(z)| \leq |z|$ and so that if $f \in Q(H)$ (respectively, is real-valued) then $F_n(f) \in Q(H)$ and $(F_n(f), HF_n(f)) \leq (f, Hf)$. Let $F_n \to F$ pointwise. Prove that for all $f \in Q(H)$, $F(f) \in Q(H)$ and $(F(f), HF(f)) \leq (f, Hf)$.

99. Let H be a Laplacian with Dirichlet or Neumann boundary conditions. Show that H satisfies the first and second Beurling–Deny criteria. (Hint: Use Problem 98 and smooth F_n approximating $|z|$ and $z \wedge 1$).

†100. Rewrite (77) in the form (76).

†101. Show that the right-hand side of (79) defines a continuous linear functional on $\{\varphi \in \mathscr{X} \mid \varphi(0) = 0 = \partial_1 \varphi(0)\}$ as long as

$$\int_{0 \leq |\lambda| \leq 1} |\lambda|^2 \, d\sigma + \int_{|\lambda| \geq 1} d\sigma < \infty$$

†102. (a) Let $f \in C_0^\infty(\mathbb{R})$ with $\int f \, dx = \int xf \, dx = 0$. Prove that there is a $g \in C_0^\infty$ with $f = g''$.
(b) Let $f \in C_0^\infty(\mathbb{R}^n)$. Write a point in $\mathbb{R}^n$ as $\langle x, y \rangle$ where $y \in \mathbb{R}$, $x \in \mathbb{R}^{n-1}$. Suppose that

$$\int f(x, y) \, dx \, dy = 0 = \int yf(x, y) \, dx \, dy$$

$$= \int x_i \, f(x, y) \, dx \, dy$$

Find functions $a_1, a_2 \in C_0^\infty(\mathbb{R}^{n-1})$, $\eta_1, \eta_2 \in C_0^\infty(\mathbb{R})$ so that

$$\int a_i(x) \, dx = \int x_j a_i(x) \, dx = 0, \qquad i = 1, 2; \quad j = 1, \ldots n - 1$$

and so that

$$g(x, y) = f(x, y) - \sum_{i=1}^{2} a_i(x)\eta_i(y)$$

obeys

$$\int g(x, y)\, dy = \int y g(x, y)\, dy = 0$$

for *each* x.

(c) Prove by induction that any f of the above form can be written as a sum $\sum_{i=1}^{n} \partial^2/\partial x_i^2\, f_i$ with $f_i \in C_0^\infty(\mathbb{R}^n)$.

(d) Prove that any $\varphi \in \mathscr{X}$ with $\varphi(0) = 0 = \partial_i \varphi(0)$ (all i) is a sum of functions of the form $\lambda_i \lambda_\ell \psi$ with $\psi \in \mathscr{X}$.

†*103.* Show that the measure $d\sigma$ defined in the proof of Theorem XIII.53 satisfies $\int_{|\lambda| \geq 1} d\sigma(\lambda) < \infty$.

†*104.* Fill in the details of Example 2 in Section XIII.13.

†*105.* Prove that any distribution solution of the radial Schrödinger equation (88) on $(0, \infty)$ with $E > 0$ is a linear combination of the two Jost solutions.

†*106.* Fill in the details in the proof of Theorem XIII.58 by making rigorous the formal calculations on $G(m, r)$.

107. Find an explicit potential V, smooth away from $r = 0$, and an eigenfunction ψ so that ψ is not in the domain of D, the infinitesimal generator of dilatations. (Hint: Modify the Wigner–von Neumann example.)

108. Let V be the sum of a repulsive potential and a homogeneous potential of degree $-\alpha$, $0 < \alpha < 2$. Prove that $-\Delta + V$ has no positive eigenvalues.

109. Let complex numbers $a_1, a_2, \ldots$ be given. Prove that there is at most one function f analytic in $\{z \mid \operatorname{Re} z > 0\}$ so that $f(n) = a_n$; $n = 1, 2, \ldots$ and $|f(z)| \leq C_1 \exp(C_2 |z|)$ for some $C_2 < \pi$. (Hint: If f_1 and f_2 are two such functions, apply Carlson's theorem to $(f_2 - f_1)/\sin \pi z$.)

110. Prove that the right-hand side of (91) is finite if $\psi \in D(-\Delta)$.

111. (a) Let $c > -\frac{1}{4}$. Let $A_c f = -f'' + cx^{-2} f$. Show that for a suitable constant d and all $\alpha \in \mathbb{R}$, $f \in C_0^\infty(0, 1)$,

$$\int_0^1 x^\alpha |f(x)|^2\, dx \leq d \int_0^1 x^\alpha |(A_c f)(x)|^2\, dx$$

(b) Let $n \geq 3$. Let $h \in C_0^\infty(\mathbb{R}^n)$ with support in $\{x \mid 0 < |x| < 1\}$. Prove there is a constant D, independent of h, so that

$$\int |x|^\alpha |h(x)|^2\, d^n x \leq D \int |x|^\alpha |\Delta h(x)|^2\, d^n x$$

for all α.

(c) Prove Theorems XIII.63 and XIII.64 for any $n \geq 3$.

112. (a) Prove Theorem XIII.57 for $n = 2$ by appealing to the $n = 3$ results. (Hint: Take functions constant in one direction.)

(b) Prove Theorems XIII.63 and XIII.57 for $n = 2$ by proving that for any $h \in C_0^\infty(\mathbb{R}^2 \setminus \{0\})$ and $\alpha > 0$,

$$\int |x|^{-\alpha-2} |h(x)|^2 \, d^2x \leq \alpha^{-1} \operatorname{Re}\left[\int |x|^\alpha \overline{h(x)}(-\Delta h)(x) \, d^3x\right]$$

(Hint: Use the fact that $\int (|x|^{\alpha/2}h)[-\Delta(|x|^{\alpha/2}h)] \, d^2x \geq 0$.)

113. (a) Let $f \in C_0^\infty(0, 1)$. Let $g = -f'' + cx^{-2}f$ for some $c > -\frac{1}{4}$. Prove that for any α,

$$\int_0^1 r^\alpha |f'(r)|^2 \, dr \leq \int_0^1 r^\alpha |g(r)|^2 \, dr$$

*(b) Prove that for $n \geq 3$ and any h that is C^∞ and supported in $\{x \mid 0 < |x| < 1\}$,

$$\int |x|^\alpha |\nabla h|^2 \, dx \leq 2 \int |x|^\alpha |\Delta h|^2 \, dx$$

(c) Prove a unique continuation theorem for Schrödinger operators with magnetic fields. Reference: The paper of Heinz quoted in the Notes.

(d) Complete the proof Theorem XIII.62.

114. Prove that a closed subset of a metric space is compact if and only if, for any ε, it can be covered by finitely many ε-balls.

115. Let A be the self-adjoint extension with periodic boundary conditions of $i\, d/dx \restriction C_0^\infty(-\pi, \pi)$ on $L^2(-\pi, \pi)$. Prove directly that the set

$$S = \{\psi \in L^2(-\pi, \pi) \mid \|\psi\| \leq 1, \|A\psi\| \leq 1\}$$

is compact.

**116.* Provide an alternative proof of Theorem XIII.65 as follows:

(a) Let $H(p) = \min\{|p|, \operatorname{ess\,min}_{|q| \geq \frac{1}{2}p} \sqrt{G(q)}\}$. Prove that for $\psi \in S$, the set given in Theorem XIII.65, and $\eta \in C_0^\infty(\mathbb{R}^n)$, one has

$$\int H(p)^2 |\widehat{\eta\psi}(p)|^2 \, dp \leq (2\pi)^n 4\left(\int (1 + 2|p|)|\hat{\eta}(p)| \, dp\right)^2$$

(Hint: Prove that $H(a + b) \leq 2|a| + \sqrt{G(b)}$.)

(b) Choose R and η supported in the box of side R, so that if $\psi \in S$ and $\psi_1 \equiv \eta\psi$, then $\|\psi - \psi_1\|_2 \leq \varepsilon/4$.

(c) Choose $R_0 > R$, so that for $|k_i| \leq \pi/R_0$ and $\varphi_k(x) \equiv e^{-ik \cdot x}\psi_1(x)$, $\|\varphi_k - \psi_1\| \leq \varepsilon/4$.

(d) Let $a_m(k)$ be the Fourier *series* coefficients for φ_k as a function in the box of side R_0. Prove that for some constant C_1, independent of $\psi \in S$,

$$\sum_m \int_{|k_i| \leq \pi/R_0} H\left(k + \frac{2\pi m}{R_0}\right)^2 |a_m(k)|^2 \, dk \leq C_1$$

(e) Find C_2, independent of $\psi \in S$, and some k, so that $\|\varphi_k - \psi\| \leq \varepsilon/2$ and

$$\sum_m H\left(\frac{2\pi}{R_0}(|m| - 1)\right)^2 |a_m(k)|^2 \leq C_2$$

Let $\psi_2 = \varphi_k$ for this special value of k.

(f) Find N independent of ψ so that a truncated Fourier series ψ_3 for ψ_2 obeys $\|\psi_2 - \psi_3\| \leq \varepsilon/4$.
(g) Complete the proof.

117. Prove Rellich's criterion as a corollary of Reisz' criterion.

118. Let $S \subset \ell_p$, $1 \leq p < \infty$. Prove that S is compact if and only if: (1) $\sup_{f \in S} \|f\|_p < \infty$; and (2) for any ε, there is an N with $\sum_{|n| \geq N} |f_n|^p \leq \varepsilon$ for all $f \in S$.

119. (Strichartz theorem, form version) Let $s \geq 3$. Prove the following results for multiplication operators W on $L^2(\mathbb{R}^3)$.

(a) If $W \in L^s_w$, then

$$\|W(I - \Delta)^{-1/2}\varphi\|_2 \leq C\|W\|_{s/2,\,w}\|\varphi\|_2$$

(b) If $V \in L^{s/2}_w$, then V is a form-bounded perturbation of $-\Delta$.
(c) If $V \in L^{s/2}$, then the relative bound is zero.

120. Prove Theorem XIII.68 by proving that each term in the Neumann series for the perturbed resolvent is compact.

†*121.* Provide the details of the proof of Theorem XIII.70.

122. Prove that if A and B are positive self-adjoint operators on a Hilbert space $\mathscr{H}$ with $B << A$, then for any closed subspace $\mathscr{H}_0$ of $\mathscr{H}$ with $\mathscr{H}_0 \cap D(A)$ dense in $\mathscr{H}_0$, $B_0 << A_0$ where A_0 and B_0 are the Friedrichs extensions of $A \restriction \mathscr{H}_0$ and $B \restriction \mathscr{H}_0$.

123. The purpose of this problem is to provide an alternative proof of Theorem XIII.73.
(a) Prove that it is sufficient to show that if $f_n \in C_0^\infty(\Omega)$ and $\|f_n\|_m \leq 1$, then $\{f_n\}$ has a subsequence convergent in the $\|\cdot\|_j$ norm.
(b) Let $f_n \in C_0^\infty(\Omega)$ satisfy $\|f_n\|_m \leq 1$. Show that $\sup_k |\hat{f}_n(k)| \leq c_0$ and that $\{f_n\}$ has a subsequence $\{f_{n_i}\}$ that converges weakly in $L^2(\Omega)$.
(c) Prove that $\hat{f}_{n_i}$ converges pointwise.
(d) Show that there are constants c_1 and c_2 so that for any $r > 0$,

$$\|f_{n_i} - f_{n_\ell}\|_j^2 \leq c_1 \int_{|k| \leq r} |k|^{2j} |\hat{f}_{n_i}(k) - \hat{f}_{n_\ell}(k)|^2 \, dk$$

$$+ c_2 r^{2j-2m} \int_{|k| \geq r} |k|^{2m} |\hat{f}_{n_i}(k) - \hat{f}_{n_\ell}(k)|^2 \, dk$$

(e) Use the inequality in (d) to conclude the proof of Theorem XIII.73.

124. (a) Prove the first part of Corollary 2 to Theorem XIII.74 by establishing the bound

$$((\eta u), (-\Delta_D)(\eta u)) \leq C[(u, (-\Delta_D)u) + (u, u)]$$

for fixed $\eta \in C_0^\infty$ identically one in a neighborhood of K.
(b) Prove the second part of Corollary 2 to Theorem XIII.74 by using the bound $x^{-2} \leq C(-\Delta)$ to control $\|\eta u_n\|$.
(c) Prove Corollary 2 to Theorem XIII.75 by showing that $(\eta, (-\Delta_N)\eta)$ and (η, η) being bounded (respectively, $\|\Delta_N u_n\|$ and $(\eta, (-\Delta_N)\eta)$ being bounded) implies bounds on the H^1 norm of η (respectively, $\nabla\eta$).

Remark The proof of the second part of (c) will require estimating $\|\partial_i \partial_j \varphi\|$ by $\|-\Delta_N \varphi\|$. Such estimates are discussed in the book of Agmon quoted in the Notes to Section 14.

125. (a) Let ∂_i be the operator closure of the ith partial derivative defined on $C_0^\infty(\Omega)$, viewed as an operator on $L^2(\Omega)$. Let ∂_i^* be its adjoint. Prove that for any open set $\Omega \subset \mathbb{R}^n$, $-\Delta_D = \sum_{i=1}^n \partial_i^* \partial_i$.

(b) For any open set $\Omega \subset \mathbb{R}^n$, prove that $-\Delta_N^\Omega = \sum_{i=1}^n \partial_i \partial_i^*$.

126. Prove Proposition 1 of Section 15 by proving the one-dimensional case and then appealing to the theory of tensor products.

127. Let C be the operator $-d^2/dx^2$ on $L^2[a, b]$ with the boundary conditions

$$\frac{df}{dx}(a) + \alpha f(a) = 0, \qquad -\frac{df}{dx}(b) + \beta f(b) = 0$$

(a) Prove that $Q(C) = H^1(a, b)$.

(b) Prove that for $f \in C^\infty(a, b)$,

$$(f, Cf) = \int_a^b \left|\frac{df}{dx}\right|^2 dx + \alpha |f(a)|^2 + \beta |f(b)|^2$$

128. (a) Let Ω be a contented set. Prove that Ω is Lebesgue measurable in the sense that there are Borel sets D_1, D_2 with $D_1 \subset \Omega \subset D_2$ so that $\mu(D_2 \triangle D_1) = 0$. (Hint: Let D_1 (respectively D_2) be a union (respectively, intersection) of inner approximating cubes (respectively, outer cubes).)

(b) Find an open Lebesgue measurable set that is discontented.

129. Let A and B be semibounded self-adjoint operators and let $\tilde{N}_E(A)$ be the number of eigenvalues of A less than $-E$.

(a) Prove that

$$\tilde{N}_E(A + B) \leq \tilde{N}_{\theta E}(A) + \tilde{N}_{(1-\theta)E}(B)$$

for $0 \leq \theta \leq 1$.

(b) Let $\tilde{S}_\gamma(A)$ be the sum of the γth powers of the negative eigenvalues of A. Prove that for $\gamma > 0$ and $0 < \theta < 1$,

$$\tilde{S}_\gamma(A + B) \leq \theta^{-\gamma} \tilde{S}_\gamma(A) + (1 - \theta)^{-\gamma} \tilde{S}_\gamma(B)$$

(Hint: Prove and use the formula $\tilde{S}_\gamma(A) = \gamma \int_0^\infty E^{\gamma-1} \tilde{N}_E(A)\, dE$.)

130. Consider the formula

$$\lim_{\lambda \to \infty} S_\gamma(\lambda V)/\lambda^{\frac{1}{2}m+\gamma} = \tau_m (2\pi)^{-m/2} \int |V_-(x)|^{\frac{1}{2}m+\gamma}\, d^m x \tag{209}$$

where $S_\gamma(W)$ is the sum of the γth powers of the negative eigenvalues of $-\Delta + W$.

(a) Prove (209) for any $V \in C_0^\infty(\mathbb{R}^n)$ by using Dirichlet–Neumann bracketing.

(b) Extend (209) for $n \geq 3$ to any $V \in L^{\frac{1}{2}m+\gamma}(\mathbb{R}^m)$.

(c) Extend (209) to $n = 1, 2$ to any $V \in L^{\frac{1}{2}m+\gamma}(\mathbb{R}^m)$ if $\frac{1}{2}m + \gamma > 1$.

(Hint: In (b) and (c) use Problem 129 and the Lieb–Thirring bounds (Problems 31–33).)

†*131.* Prove Theorem XIII.82.

132. Let W be such that $\dim E_{(-\infty, 0]}(-\Delta + \lambda W) < \infty$ for all λ. Suppose that

$$f(\lambda) \equiv \lim_{a \downarrow 0} [\dim E_{(-\infty, \lambda a]}(-\Delta + \lambda V)/\dim E_{(-\infty, a]}(-\Delta + V)]$$

exists for all λ and is finite, that

$$\lim_{a \uparrow 0} E_{(-\infty, a]}(-\Delta + V) = \infty$$

and that $f(\lambda)$ is continuous at $\lambda = 1$. Prove that

$$\lim_{a \uparrow 0} [\dim E_{(-\infty, a]}(-\Delta + V + W)/\dim E_{(-\infty, a]}(-\Delta + V)] = 1$$

(Hint: First prove that if $\dim E_{(-\infty, 0]}(B) = N < \infty$, then $\dim E_{(-\infty, a]}(A + B) \leq \dim E_{(-\infty, a]}(A) + N$.)

133. Verify the properties of $A_1 \oplus A_2$ appearing before Proposition 3 in Section 15.

134. Let $f_n \in L^2(M, d\mu; \mathscr{H}') = \mathscr{H}$ where $\mathscr{H}'$ is a separable space and M is σ-finite. Suppose that $\{f_n(m)\}_{n=1}^{\infty}$ is an orthonormal basis for $\mathscr{H}'$ for almost all $m \in M$. Prove that

$$\sum_{n=1}^{N} (f_n(\cdot), f(\cdot))_{\mathscr{H}'} f_n(\cdot) \to f$$

in $\mathscr{H}$ for each $f \in \mathscr{H}$. (Hint: Use the monotone convergence theorem.)
Remark This extends Problem 12 of Chapter II.

135. Suppose that A is a self-adjoint operator. Let $U(t)$ be a unitary one-parameter group. Suppose that $\mathscr{D}$ is a core for A and that $U(t)\mathscr{D} \subset \mathscr{D}$ with $AU(t)\psi = U(t)A\psi$ for all t and all $\psi \in \mathscr{D}$. Prove that $U(t)D(A) = D(A)$ and that $U(t)e^{iAs} = e^{iAs}U(t)$.

†*136.* (a) Prove (b) of Theorem XIII.85.
(b) Fill in the details in the proof of (c) of Theorem XIII.85.

137. Prove that the Fourier transform of $(2\pi)^{-1/2}(p^2 + 1)^{-1}$ is $\frac{1}{2}e^{-|x|}$. (Hint: Use contour integration.)

138. Let $f \in \mathscr{S}(\mathbb{R})$ and define

$$V(x) = \sum_{n=-\infty}^{\infty} f(x + 2\pi n)$$

(a) Using the theory of Fourier transforms of periodic distributions, (144) and (145), prove that

$$\hat{V}(k) = \sum_{n=-\infty}^{\infty} \hat{f}(n)\, \delta(k - n)$$

(b) Using the Fourier inversion formula for $V(0)$ prove the **Poisson summation formula**

$$\sum_{m=-\infty}^{\infty} f(2\pi m) = (2\pi)^{-1/2} \sum_{n=-\infty}^{\infty} \hat{f}(n)$$

(c) Suppose that f and $\hat{f}$ are continuous functions with $|f(x)| \leq C(1 + |x|)^{-1-\delta}$ and $|\hat{f}(k)| \leq C(1 + |k|)^{-1-\delta}$ for some $C, \delta > 0$. Prove the Poisson summation formula for f by a limiting argument.
(d) Using the known Fourier transform of $e^{-|x|}$, evaluate $\sum_{n=-\infty}^{\infty} (1 + n^2)^{-1}$.
(e) Using the known Fourier transform of $e^{-\alpha|x|}$, evaluate $\sum_{n=1}^{\infty} n^{-2}$.

Remark As the above suggests, the Poisson summation formula is a useful tool in number theory, see for example, K. Chandrasekhar, *Introduction to Analytic Number Theory*, Springer-Verlag, Berlin and New York, 1968.

139. (The Krönig–Penny model) Let V be the potential of period 2π which is 0 on $[0, y)$ and c on $[y, 2\pi)$. Compute the discriminant explicitly and prove that as $n \to \infty$, the size of the nth gap obeys

$$\ell_n \sim \left| \frac{4c}{n} \sin\left(\frac{ny}{2}\right) \right|$$

In particular, conclude that infinitely many gaps occur.

†*140.* Let A be a decomposable self-adjoint operator on $\mathscr{H} = \int_M^{\oplus} \mathscr{H}' \, d\mu$. Suppose that each $A(m)$ is bounded from below and has compact resolvent.

(a) Prove that $E_n(m)$, the nth eigenvalue of $A(m)$, is a measurable function. (Hint: Use the min–max principle.)

(b) Show that $\mathscr{H}'$-valued functions $\psi_n(m)$ can be chosen which obey $A(m)\psi_n(m) = E_n(m)\psi_n(m)$ and which are an orthonormal basis of $\mathscr{H}'$ in such a way that the $\psi_n(\cdot)$ are measurable. (Hint: For given n, let $M_{k;n} = \{m \,|\, E_n(m) \text{ is } k\text{-fold degenerate}\}$ and choose $\psi_n(m)$ on each $M_{k;n}$.)

(c) Suppose also that M is a topological space, that each $A(m) > 0$, and that $(A(m) + 1)^{-1}$ is norm continuous. Prove that $E_n(m)$ is continuous.

(d) Give an example where $(A(m) + 1)^{-1}$ is weakly continuous and $E_n(m)$ is not continuous.

(e) Explain why $\psi_n(m)$ may not be continuous even under the hypotheses of (c).

†*141.* (a) Verify (173b).

(b) Let $\alpha > \frac{1}{2}n$. Verify that

$$\sum_{|m| \geq c_2(1+|y|)} |E_m(x + iy) + 1|^{-\alpha} \leq c_3(1 + |y|)^{-\alpha + \frac{1}{2}n}$$

(c) Let $\alpha > 1$. Verify that

$$\sum_{|m| \leq c_2(1+|y|)} |E_m(x + iy) + 1|^{-\alpha} \leq c_4(1 + |y|)^{-\alpha + n - 1}$$

(d) Conclude the proof of Lemma 1 to Theorem XIII.100.

142. Prove that any lattice in $\mathbb{R}^n$ has a basis.

143. Prove that the Wigner–Seitz cell of any lattice is a polyhedron, i.e., an intersection of finitely many half spaces. (Hint: Let $\mathbf{a}_1, \ldots, \mathbf{a}_n$ be a basis and let V be the set of 3^n points $\sum_{i=1}^n t_i \mathbf{a}_i$ with $t_i = 0, +1$, or -1. Let $R = \max\{|x| \,|\, x \in V\}$ and prove that any point in C, the Wigner–Seitz cell, is in the ball of radius R. Prove that a point on ∂C is equidistant from 0 and some point in $\mathscr{L} \cap \{x \,||x| \leq 2R\}$.)

144. Suppose that A_α is a family of self-adjoint operators, bounded from below, such that $A_\alpha \geq A$ and that A has compact resolvent. Let $E_n(\alpha)$ be the nth eigenvalue of A_α. Prove that $E_n(\alpha) \to \infty$ uniformly in α as $n \to \infty$.

145. Prove that the density of states measure given by (176) is absolutely continuous with respect to Lebesgue measure. (Hint: Prove that it is a sum of spectral measures for H.)

146. In the one-dimensional case prove that at a point E with $E_n(k) = E$ the density of states is given by

$$\frac{d\rho}{dE} = \frac{2}{|\tilde{Q}|}\left(\frac{dE}{dk}\right)^{-1}$$

†*147.* Fill in the details of the proof of Theorem XIII.101.

**148.* Prove the analogue of Theorem XIII.101 when periodic boundary conditions are replaced by Dirichlet or Neumann boundary conditions.

149. Using (185), prove (186).

150. Let $\sum_{i=1}^{\infty} |a_i| < \infty$. Let $f_N(z) = \prod_{j=1}^{N} (1 + a_j z)$. Prove that f_N converges as $N \to \infty$ uniformly on compact sets as follows:
(a) Prove uniform bounds on $f_N(z)$ by using $|1 + x| \leq e^{|x|}$.
(b) Prove that the Taylor coefficients of f_N converge as $N \to \infty$.
(c) Complete the proof of convergence.

151. (a) Let $A_n \to A$ in trace class norm and suppose that $\mu \notin \sigma(A)$. Prove directly (without use of Theorem XIII.107) that

$$\det(1 + \mu A_n)(1 + \mu A_n)^{-1} \to \det(1 + \mu A)(1 + \mu A)^{-1}$$

in norm.
(b) Prove (196) knowing it is true when A is finite rank with $\mu \notin \sigma(A)$.

152. Let $d(\mu) = \det(1 + \mu A)$ and $D(\mu) = d(\mu)(1 + \mu A)^{-1}A$. Write $d(\mu) = \sum_{n=0}^{\infty} a_n \mu^n$ and $D(\mu) = \sum_{n=0}^{\infty} B_n \mu^n$.
(a) Prove that $|a_n| \leq (e/n)^n \|A\|_1^n$.
(b) Prove that $\|B_n\|_1 \leq (e/n)^n \|A\|_1^{n+1}$.

153. Define the **partial trace** Tr_{n-1} from $\mathscr{I}_1(\bigotimes^n \mathscr{H})$ to $\mathscr{I}_1(\mathscr{H})$ by $\mathrm{Tr}(C\,\mathrm{Tr}_{n-1}(A)) = \mathrm{Tr}[(C \otimes I \otimes \cdots \otimes I)A]$ for any $C \in \mathscr{L}(\mathscr{H})$.
(a) Show that Tr_{n-1} is a well-defined contraction.
*(b) View $\bigwedge^k(A)$ as a map on $\bigotimes^k \mathscr{H}$ by setting it equal to zero on $(\bigwedge^k \mathscr{H})^{\perp}$. Prove that $D(\mu) = \sum_{n=0}^{\infty} B_n \mu^n$ with

$$B_n = (n + 1)\mathrm{Tr}_n(\bigwedge^{n+1}(A))$$

154. Prove that $|\lambda_1(A) \cdots \lambda_n(A)| \leq \mu_1(A) \cdots \mu_n(A)$ for any compact A. (Hint: Consider the eigenvalues and norm of $\bigwedge^n(A)$.)

155. Let $A \in \mathscr{I}_p$ with $p \leq n$. Define

$$R_n(A) = (1 + A)\exp\left(\sum_{k=1}^{n-1} (-A)^k/k\right) - 1$$

(a) Prove that $R_n(A) \in \mathscr{I}_1$.
Define $\det_n(1 + A) = \det(1 + R_n(A))$.
(b) Prove that $1 + A$ is invertible if and only if $\det_n(1 + A) \neq 0$.
(c) Prove that

$$\det_n(1 + A) = \prod_{j=1}^{N(A)} \left[(1 + \lambda_j(A))\exp\left(\sum_{k=1}^{n-1} (-\lambda_j(A))^k/k\right)\right]$$

Let $D_n(\mu A) = A(1 + \mu A)^{-1} \det_n(1 + \mu A)$.

*(d) Prove that

$$|\det_n(1 + A)| \leq \exp(\gamma_n \|A\|_n^n)$$

$$\|D_n(\mu A)\|_n \leq C_n \exp(\gamma_n \|A\|_n^n \mu^n)$$

for suitable constants C_n and γ_n.

(e) Find Plemelj–Smithies formulas for $\det_n$ and D_n.

(f) Find completeness criteria for eigenvectors of operators in $\mathscr{I}_n$.

156. Prove that the following are equivalent for $A \in \mathscr{I}_1$:

(a) A is quasi-nilpotent, i.e., $\sigma(A) = \{0\}$.

(b) $\det(1 + \mu A) = 1$.

(c) $\operatorname{Tr}(A^k) = 0$ for all $k > 0$.

(d) $\operatorname{Tr}(A^k) = 0$ for all $k > k_0$ for some k_0.

157. Prove the following are equivalent for all $A \in \mathscr{I}_1$:

(a) For all $\mu \in \mathbf{C}$, μ and $-\mu$ have identical algebraic multiplicities.

(b) $\det(1 + \mu A) = \det(1 - \mu A)$ for all $\mu \in \mathbb{C}$.

(c) $\operatorname{Tr}(A^k) = 0$ for all odd k.

†*158.* (a) Prove the max–min principle for singular values:

$$\mu_n(A) = \inf_{\psi_1, \ldots, \psi_{n-1}} \left(\sup_{\phi \in [\psi_1, \ldots, \psi_{n-1}]^\perp;\ \|\phi\| = 1} \|A\phi\| \right)$$

(b) Prove that $\mu_n(1 + A) \leq 1 + \mu_n(A)$.

(c) Prove **Fan's inequality**

$$\mu_{n+m+1}(A + B) \leq \mu_{n+1}(A) + \mu_{m+1}(B)$$

†*159.* Let A be a closed operator and let $\mu \notin \sigma(A)$ and P be the spectral projection for some isolated point λ in $\sigma(A)$. Prove that P is also the spectral projection associated to the operator $(A - \mu)^{-1}$ and the point $(\lambda - \mu)^{-1}$.

160. Let D be a bounded open set in $\mathbb{R}^{n+1}$ with smooth boundary ∂D. Let $\mathscr{H} = L^2(\partial D, dS)$. Let $K(x, y)$ the kernel of an integral operator A on $\mathscr{H}$ and suppose that

$$|K(x, y)| \leq C|x - y|^{-\alpha}$$

with $\alpha < n$. Suppose that L is the kernel of an integral operator B, with

$$|L(x, y)| \leq D|x - y|^{-\beta}$$

(a) If $\alpha + \beta < n$, prove that AB has a bounded kernel.

(b) If $\alpha + \beta > n$, prove that AB has a kernel M with

$$|M(x, y)| \leq E(x - y)^{-\gamma}$$

$\gamma = \alpha + \beta - n$.

(c) Let $\alpha < n[1 - (2k)^{-1}]$, for k equal a positive integer. Prove that $A \in \mathscr{I}_{2k}$.

*(d) Let $2 \leq p < \infty$. Let $\alpha < n(1 - p^{-1})$. Prove that $A \in \mathscr{I}_p$. (Hint: Use complex interpolation.)

161. (a) Let $f \in L^2(\mathbb{R})$ have an L^2 derivative. Prove that there are $g, h \in L^2$ with $f = g * h$.
(b) Let $f \in L^2(\mathbb{R})$ have an L^2 derivative; $V, W \in L^2(\mathbb{R})$. Prove that

$$V(x)f(x-y)W(y)$$

is the kernel of a trace class operator on $L^2(\mathbb{R})$.
(c) Let $V, W \in L^2(\mathbb{R})$ have *compact support*. Let f be *locally* L^2 with a *locally* L^2 derivative. Prove that

$$V(x)f(x-y)W(y)$$

is the kernel of a trace class operator.

162. Let B be a rank one operator. Prove that $\det(1+B) = 1 + \mathrm{Tr}(B)$. (Hint: Replace B by λB and prove it for small λ.)

163. (a) Prove that the Fourier transform of the distribution $|x|$ on $\mathbb{R}$ is a distribution equal to the function $-(2/\pi)^{1/2}k^{-2}$, away from $k = 0$.
(b) Prove that $-|x|$ is conditionally strictly positive definite; i.e., if $(1+|x|)V \neq 0$ is in L^1 and $\int V(x)\,dx = 0$, then

$$-\int V(x)|x-y|V(y)\,dx\,dy > 0$$

164. Suppose that A and B are trace class operators with $A \geq 0$.
(a) Prove that $|B|^{1/2}(1+\mu A)^{-1/2}$ converges to zero in Hilbert–Schmidt norm as $\mu \to \infty$. (Hint: Compute $\mathrm{Tr}((1+\mu A)^{-1/2}|B|(1+\mu A)^{-1/2})$ in an eigenbasis for A.)
(b) Prove that $B(1+\mu A)^{-1}$ converges to zero in trace class norm as $\mu \to \infty$.
(c) Prove that $\lim_{\mu\to\infty}[\det(1+B+\mu A)/\det(1+\mu A)] = 1$; where det is the Fredholm determinant.

165. Consider the one-dimensional Schrödinger operator $-d^2/dx^2 + V(x)$ with V positive and periodic with period 1. Let $D(E)$ be the discriminant for this equation and $D_0(E) = 2\cos\sqrt{E}$, the discriminant for $V = 0$. Let G_0 be the inverse of $(h_0+1)^{-1}$ with h_0 the operator $-d^2/dx^2$ on $L^2(0,1)$ with periodic boundary conditions. Prove that

$$D(E) - 2 = C[\det(1 + G_0V - (E+1)G_0)]$$

where det is the Fredholm determinant and

$$C = D_0(-1) - 2$$

(Hint: First prove that $D(E) - 2 = C_V[\det(1 + G_0V - (E+1)G_0)]$ by showing that both sides are entire functions given as infinite products and that they have the same zeros. Then, using Problem 164, prove that $C_V = C_0$ by showing that $(D(E)-2)/(D_0(E)-2)$ and $\det(1+G_0V-(E+1)G_0)/\det(1-(E+1)G_0)$ approach one as $E \to -\infty$. Find C_0 by taking $E = -1$.)

166. Let E and F be two bounded operators.
(a) Suppose that $0 \neq \lambda \notin \sigma(EF)$. Prove that $-(\lambda)^{-1}[1 - F(EF-\lambda)^{-1}E]$ is a two-sided inverse for $FE - \lambda$ and conclude that $\lambda \notin \sigma(FE)$.
(b) Let $\lambda \neq 0$, and $\mathcal{M} = \{\varphi \mid EF\varphi = \lambda\varphi\}$; $\mathcal{N} = \{\varphi \mid FE\varphi = \lambda\varphi\}$. Prove that F is a bijective map of $\mathcal{M}$ onto $\mathcal{N}$ and conclude that $\dim \mathcal{M} = \dim \mathcal{N}$.

167. Let $p \neq \infty$. Suppose that $A_n \in \mathscr{S}_p$ with $\sup_n \|A_n\|_p < \infty$ and let A be a bounded operator with $A_n \to A$ weakly. Prove that $A \in \mathscr{S}_p$ and $\|A\|_p \leq \varliminf \|A_n\|_p$. (Hint: Let q be the dual index to p. Prove that $|\mathrm{Tr}(FA)| \leq \|F\|_q \varliminf \|A_n\|_p$ for any finite rank operator F.)

168. Prove the bound $\|C^{1/2}DC^{1/2}\|_r \leq \|CD\|_r$ used in the proof of the generalized Golden–Thompson inequality by using complex interpolation.

169. This problem asks the reader to prove Hölder's inequality for matrices (Proposition 5 of the appendix to Section IX.4) from Hölder's inequality for sums without recourse to complex interpolation.

(a) Let $\{a_{ij}\}_{1 \leq i,\, j \leq n}$ be a matrix with $\sum_i |a_{ij}| \leq 1$ for all j and $\sum_j |a_{ij}| \leq 1$ for all i. Prove that

$$|\sum a_{ij}\mu_i \nu_j| \leq \left(\sum_i |\mu_i|^p\right)^{1/p} \left(\sum_j |\nu_j|^q\right)^{1/q}$$

for $p^{-1} + q^{-1} = 1$. (Hint: Look at the proof of Theorem XIII.103.)

(b) Let $A = \sum \mu_i(\varphi_i, \cdot)\psi_i$ and $B = \sum \nu_j(\eta_j, \cdot)\gamma_j$ be the canonical expressions for A and B. Prove that

$$|\mathrm{Tr}(AB)| \leq \sum |a_{ij}|\mu_i \nu_j$$

where $\sum_i |a_{ij}| \leq 1$, $\sum_j |a_{ij}| \leq 1$.

(c) Conclude that $|\mathrm{Tr}(AB)| \leq \mathrm{Tr}(|A|^p)^{1/p}\, \mathrm{Tr}(|B|^q)^{1/q}$.

170. Let $F_A(\mu)$ be the function of Theorem XIII.107. The purpose of this problem is to show that for fixed $A, B \in \mathscr{S}_1$, the function $\lambda \mapsto F_{A+\lambda B}(1)$ is entire in λ. This is needed to prove (197).

(a) Fix μ with $-\mu^{-1} \notin \sigma(A)$. Show that $F_{A+\lambda B}(\mu) = F_C(\lambda)F_A(\mu)$ where $C = \mu(1 + \mu A)^{-1}B$ and conclude that $\lambda \mapsto F_{A+\lambda B}(\mu)$ is entire for such μ.

(b) Let $\mu_n \to \mu_\infty$ and let $f_n(\lambda) = F_{A+\lambda B}(\mu_n)$. Using the first part of the proof of Theorem XIII.107, show that

$$\sup_n \sup_{\lambda \in R} |f_n(\lambda)| < \infty$$

for any bounded region R and that $f_n(\lambda) \to f_\infty(\lambda)$ for each λ. Conclude that $F_{A+\lambda B}(\mu)$ is entire in λ for fixed μ.

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r (radius of gyration) 197
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