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Encyclopedia of Mathematical Physics

Introductory Articles

数学物理学百科全书 1

数学物理学导言

Jean-Pierre Françoise, Gregory L. Naber, Tsou Sheung Tsun

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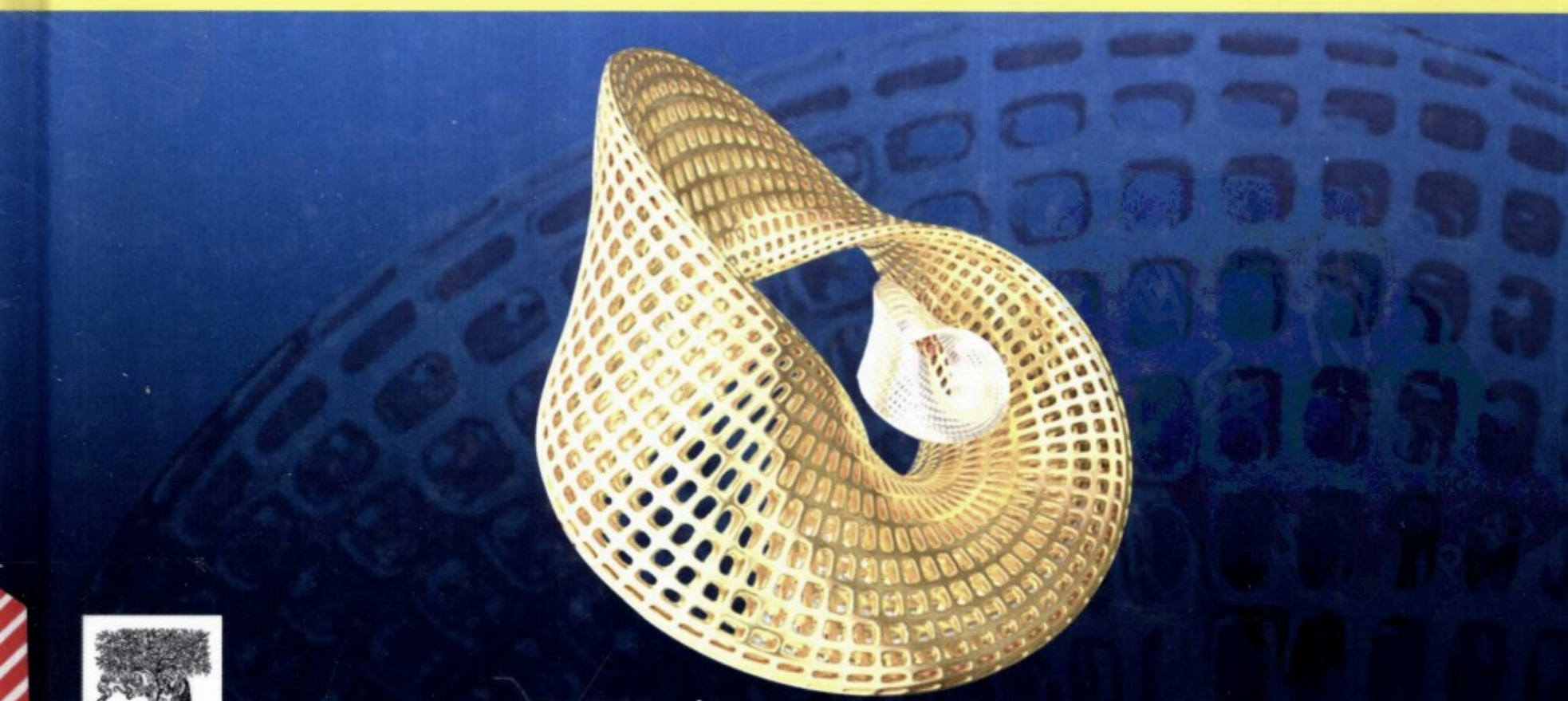

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《数学物理学百科全书》导读版编委会

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导　读

“数学物理”是基于数学和物理学这两大基础学科，经过长期相互交叉融合而逐渐形成的一个重要研究领域。物理学与数学是人类探索大自然现象和变化规律发展起来的两门最基本的学科，起源于人类早期的生产实践活动。古时欧洲学者把物理学当作“自然哲学”，“物理”一词最先出自的希腊文原意是指“自然”。随着人们对自然界认识的深入，物理学从哲学中逐渐分离出来成为一门独立的学科，并在近代得到前所未有的迅猛发展，为人类文明和社会进步提供了最基本和最丰富的科学思想和研究手段，成为自然科学的基础。物理学研究的对象是宇宙的基本组成要素：物质、能量、空间、时间，以及它们的相互作用和基本结构及其运动规律。数学被古希腊学者视为哲学之起点，“数学”一词的希腊语意思是“学问的基础”，数学亦被中国古代当作六艺之一，在由计数、计算、量度，以及对物体形状和运动的观察中产生和形成。数学研究的概念是透过抽象化和逻辑推理反映自然界的基本特征：数量、结构、变化及它们的相互关系和空间形式。

物理学作为构成自然科学的基础，而它的理论通常又以数学的形式表达出来。随着各学科向着综合和交叉方向的发展，“数学物理”的研究在近几十年取得了巨大的进展，正发展成具有特色的一门交叉学科。尽管对它的刻画还不很清晰，但总体来说，“数学物理”研究的是以物理基本问题为对象的数学理论和数学方法，寻求物理现象的数学描述和物理理论的数学结构，探究理论模型中物理问题的数学解法和解析结果，探讨理论上自洽的数学物理模型，力求解释和预言自然界的物理现象。

开展对“数学物理”的深入研究，有助于揭示出物理学与数学之间的内在联系。事实上，从自然哲学发展到物理学，除了使用实验手段和新的思维方法，数学起了不可替代的作用。当人们通过分析大量实验数据和吸取各种唯象理论的精髓，以严格的数学语言和简洁的数学公式描述支配物质基本结构和宇宙演化的物理规律时，物理学的简洁美、统一美、对称与不对称美则通过深刻的数学美反映出来。可以说，自从物理学成为自然科学的一门独立学科后，物理学与数学之间的关系变得密不可分。古代的许多科学家既是数学家也是物理学家，尤其到了近代和现代，许多理论物理学家对数学的运用和发展起到了更为积极的推进作用，数学家和理论物理学家之间的合作也变得越来越平凡、越来越深入，他们成为了“数学物理”的践行者。大家最为熟知的古希腊的阿基米德，他既是著名的数学家也是著名的物理学家，他很早就利用数学这个工具证明了杠杆定理和浮力定理，并做了大量的实验。牛顿在研究物体和天体的运动规律时发展出新的数学方法——微积分。爱因斯坦则运用对当时的物理学家来说全新的数学方法——微分几何和黎曼几何，创立了广义相对论。狄拉克推导得到的关于自旋为 1/2 的电子波函数方程预言了反粒子的存在。Yang-Mills 规范场的大范围整体性质和手征量子反常与纤维丛的拓扑不变量和 Chern-Simons 示性类及指标定理之间建立起直接的联系。超弦理

论中的额外维空间与 Calabi-Yau 空间之间的对应关系。理论物理学家 Witten 在发展超弦理论的同时由于对数学的杰出贡献而获得菲尔兹奖。这些都是物理学与数学相互结合所呈现在“数学物理”方面的经典例子。

随着物理学和数学的深入发展，“数学物理”的研究内容变得越来越丰富，新的研究结果和方法及新的观点以越来越快的速度不断呈现。同时，数学物理的新进展使得解决物理问题的能力增强，并对数学的发展起到积极的促进作用。数学物理中的许多方法和结果及数学模型已越来越多地渗透和应用到其他各门科学，如化学、天文学、地学、生物学、经济学等。数学物理对技术的进步也发挥着越来越重要的作用，为精确地求解工程技术中遇到的物理问题和数值计算提供新的方法。

20 世纪，物理学被公认为科学技术发展中最重要的带头学科，以物理学和数学为基础的“数学物理”得到了快速发展。21 世纪科学技术的发展趋势更是日新月异，人类文明和社会进步面临着各种新的挑战，如全球变暖和能源环境等问题。为此，进一步提高认识自然和改造自然的能力仍将是人类探索和研究自然界的共同目标，物理学和数学在本世纪将继续起着重要的基础作用，“数学物理”作为基础学科将进一步显示其独特优势，并取得新的更大进展。面对这样的机遇和挑战，拥有一本搜集整理数学物理全面知识的百科全书，以便更好地了解近代和现代物理学与数学方面的重大进展，掌握数学物理的基本方法，是所有在这个领域开展研究和对这个领域感兴趣的科技工作者和青年学生的迫切愿望。

由衷感谢 Elsevier 公司于 2006 年 6 月出版的“Encyclopedia of Mathematical Physics”(《数学物理学百科全书》)，这是一部全面介绍数学物理知识的百科全书。

本书的三位主编（法国巴黎居里大学 Jean-Pierre Françoise 教授、美国费城 Drexel 大学 Gregory L. Naber 教授和英国牛津大学 Tsou Sheung Tsun 博士）都是长期从事数学物理方面研究的知名学者。他们邀请了包括诺贝尔物理学奖获得者杨振宁教授和英国牛津大学 Roger Penrose 教授在内的 34 位著名物理学家和数学家作为本书的编辑顾问委员会成员，组织来自 30 个国家的 439 位在物理学和数学相关研究领域做出杰出贡献的理论物理学家和数学家，撰写了 400 多篇图文并茂的综述性文章。

《数学物理学百科全书》是经长达 4 年完成的一部内容全面系统、领域涵盖广泛的百科全书。全书特色鲜明，既体现了学科的基础性、独立性、完整性，又注重学科的前沿性、交叉性、应用性，是当今数学物理研究领域最新和最全的百科全书。

本书内容涉及物理学和数学的几乎各个重要研究领域，遍及从经典力学到量子力学、经典场论到量子场论、共形场论到拓扑场论、流体动力学到动力系统、可积系统到无序系统、粒子物理到天体宇宙学、相对论到量子引力、规范理论到统一理论、平衡态统计到非平衡态统计、凝聚态物质到量子信息、变分技术到代数方法、泛函分析到算子代数、路径积分到随机方法、李群到量子群、微分几何到代数拓扑、低维几何到非交换几何、复几何到辛几何等核心领域和方向。本书内容还特别注重数学物理的最新研究成果和在各领域的最新应用，并提供了大量必要的和重要的参考文献。这为有兴趣利用严密的数学框架求解物理问题和描述自然界基本规律的广大科研人员、教师和学生，提供了一部难得的数学物理资料书和实用的工具参考书，也有助于广大读者在了解和掌握物理学和数学前沿发展的基础上，进一步拓展其在交叉学科领域的应用和激发出新的研究

方向和领域。

我们真诚感谢科学出版社引进了《数学物理学百科全书》这部优秀的工具书。目前，我国的物理学和数学正进入一个快速发展的时期，为适应和满足广大科技工作者的需求，由科学出版社即将发行的《数学物理学百科全书》导读版，采取选编的形式，把以英文字母为目录编排出版的5卷一套的原版《数学物理学百科全书》重新编辑成按照学科分类的12卷一套《数学物理学百科全书》导读版小型丛书，其中基础理论导论1卷（含中文翻译），物理学方面共7卷（保持英文原版），数学方面共4卷（保持英文原版）。

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《数学物理学百科全书》第四卷：规范理论；量子场论

《数学物理学百科全书》第五卷：广义相对论；量子引力；弦论与M-理论

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第一卷为中英双语版，包含经典力学、微分几何、电磁学、平衡态统计力学、泛函分析、闵可夫斯基时空和狭义相对论、量子力学和拓扑学8篇导论性文章。这些介绍性文章主要是针对初学者和研究生，可作为他们在阅读各专业学科文章前的预备知识，如数学方面的文章针对物理研究生，物理学方面的文章针对数学研究生。这些文章也可作为高年级研究生课程的基础。

原版《数学物理学百科全书》的编辑以英文字母为目录，其结构具有整体性和交叉性，但所有不同学科领域的读者必须拥有全套5卷才能保证每一学科领域内容的相对完整性。导读版《数学物理学百科全书》则考虑各学科本身的相对独立性和完整性，同时注意相关学科之间交叉融合的特点，尽量把关联性强的学科内容编排在同一卷，并对那些基础理论性和交叉融合性强的综述文章，采用重复编排的方式收录进不同分卷，以保证每卷的相对完整性和独立性及有效的交叉性。

本书物理学部分与数学部分的关系很难分开。实际上，经典力学、电磁学、统计力学、量子力学、流体力学、可积系统和动力系统中的许多物理问题可归结为求解数学上的常微分方程、偏微分方程、积分方程、微分积分方程等数学物理方程，物理学问题的

解会涉及复变函数和特殊函数等多种函数，在求解时又会用到变分技术、调和分析、泛函分析等各种数学分析方法。同时，对爱因斯坦狭义相对论和广义相对论，它不仅改变了人们的时空观，还使得闵可夫斯基时空的几何学和黎曼空间的几何学成为物理理论的数学基础，同时也使得向量分析、张量分析和微分几何等成为必要的数学分析工具。在量子力学中，物理量成为算子，物理状态用波函数来描述，算子的谱才是测量到的物理量。在量子场论中，波函数又被二次量子化成为算子用来描述基本粒子在相互作用过程中的产生和湮灭。这使得算子代数、量子化方法和路径积分等数学理论和方法成为量子物理的数学基础。粒子物理学家发现自然界的3种基本作用力：电磁相互作用、弱相互作用和强相互作用可用规范理论来描述，并完全由规范对称性来支配，这些对称性在数学上用李群和李代数来描写。事实上，晶体的结构也是由欧几里得空间中的转动群来描述。这使得群论在物理学中的应用，尤其在粒子物理中的应用变得越来越重要。在规范理论中，规范势当作基本的量子场，而它被发现就是数学家在现代微分几何学中所研究的纤维丛上的联络，这使得有关纤维丛的拓扑不变量在粒子物理和量子场论研究中变得重要起来，如规范场的磁单极子和瞬子解及手征量子反常等。在量子引力和超弦理论的研究中，不仅运用到已有的数学理论和方法尤其是现代数学，还促进了数学理论本身的发展。同样，在凝聚态物质和光学方面，物质的拓扑相和拓扑缺陷、拓扑量子计算等也应用到了许多现代数学方法，这使得代数拓扑、代数方法、量子群、复几何、辛几何与拓扑、低维几何、非交换几何等数学理论和数学方法越来越多地渗透到理论物理的研究中。另外，在研究微观物理对象的随机性和各种随机过程的统计规律、无序系统和动力系统时，随机方法和离散数学等也得到越来越广泛的应用。

正如《数学物理学百科全书》三位主编在序言中写道："数学物理把数学和物理学这两大学科的优势集中到一起，它们的关系是共同发展。一方面，它运用数学这一工具把不断增长的精确性和复杂性这些物理概念组织了起来；另一方面，物理学家为数学家提供了灵感的源泉。"同时，也正如诺贝尔物理学奖获得者荷兰 Utrecht 大学 Gerard't Hooft 教授在前言中指出："物理世界与数学世界之间存在明显的重要区别。物理世界强调事实的'真相'，无论'真相'是什么，而数学是纯逻辑和纯推理的世界。在物理学中，一个理论是否能被接受是由实验来最后决定的。物理学中的方法论也与数学不同。"

物理学中的许多规律还有待于在更小或更大的尺度上进行检验。尤其在接近普朗克尺度的情况下，我们对量子场和时空的性质还不很清楚，包括量子场论中的无穷发散困难与正规化和重整化方法、非微扰相互作用效应等基本问题。诺贝尔物理学奖获得者美国加州大学圣巴巴拉分校卡弗里理论物理研究所 David Gross 教授在中国科学院理论物理研究所"前沿科学论坛"上所做的题为"物理学的未来"的报告中探讨了物理学面临的25个问题：

宇宙的起源：这一过去的哲学问题，产生了现在理论物理学家称为的宇宙学。宇宙学的观测表明，宇宙是不断膨胀的。这样，随着时间的倒推，宇宙将不断的收缩，利用爱因斯坦的广义相对论和粒子物理学知识，宇宙必然存在一个具有极高能量和密度的起点，即大爆炸。在这一点，我们现在的许多科学规律将失效。那么，我们希望知道宇宙是如何起源的？大爆炸是如何开始的？在大爆炸点到底发生了什么？

暗物质的本质：宇宙学的观测表明，构成宇宙的物质绝大部分并不是今天我们看到的物质，而是一些并不发生辐射的东西，即暗物质。构成宇宙的物质中大约有 25%是暗物质，而普通的物质（例如，构成我们身体的重子）只占到大约 3%。因此，什么是暗物质？我们能否在实验室中观测到它？它与普通的物质是如何发生作用的？暗物质在宇宙中是如何分布的？尽管现在人们构造了许多超出标准模型的模型来描述这种相互作用，其中有暗物质的候选者如轴子和超对称中的中性粒子，但是以上许多问题仍然不能很好的回答。

暗能量问题：宇宙中绝大部分能量是以另一种形式，即暗能量的形式存在。暗能量的本质是什么？它是个常量还是随时间变化的？如何利用实验来观测暗能量随时间的变化？对暗能量最简单的假设是爱因斯坦的宇宙学常数，这一常数是爱因斯坦在广义相对论引力方程中为了得到静止的宇宙而不是膨胀的宇宙而引入的。现在看来这一常数和暗能量有许多相似之处，但是暗能量到底与这一宇宙学常数是否是一回事有待回答。

天体的形成：星体是如何形成的？如何来理解星体的质量谱、双子星和星团的频率？如果一个星体形成理论足够好，那么它应该可以告诉我们第一个星体形成的景象，但是这样的理论并不存在。对这一问题的研究出于我们希望知道在太阳系以外的星系中是否存在生命。

广义相对论：是否现在对于广义相对论的理解在所有尺度上都是正确的？广义相对论已经被许多实验证明，确实是值得信服的。但是，目前我们还有两个地方没有检验，其一是在极小尺度上（事实上，在极小尺度上我们也没有检验牛顿引力理论），其二是在引力作用及其强的区域如黑洞的附近。由此，我们要问两个问题，一个问题是：是否强引力能够经受得住天文学引力波的检验？另一个问题是：能否用宇宙学观测量来判断 Kerr 度规是否正确地描写了黑洞周围的几何？

量子力学：量子力学是否是描述自然界的最终理论？在极大尺度、复杂体系、意识体系它是否还正确？它是否可以作为一个描述宇宙的理论？

粒子物理标准模型：标准模型是一个极其成功的理论，它包含不多的参数，与实验符合得相当好。但是它也有一些我们难以回答的神秘之处，例如，夸克和轻子的质量谱中质量的差别和质量的起源、夸克之间和轻子之间的混合、重子的起源和质子的寿命等。

超对称：超对称是对标准模型的最自然的扩充，并且考虑了超对称和超对称破缺后，各种作用可以做到很好的统一。但是，超对称是如何破缺的？是否存在低能超对称？超对称中粒子的质量谱是什么等一系列问题还有待解决。

量子色动力学：我们是否能够求解量子色动力学？如果我们设想夸克的颜色数是无穷大而不等于 3，是否能够构造一个强子的弦论对偶描述？

弦论：弦论是一个有希望统一所有相互作用的理论。但是，什么是弦论？弦论中存在大量的对偶性会给我们什么启示？

时空概念：什么是时空？时空的概念是否是必然存在的？不同的理论物理学家有不同的观点，例如，美国普林斯顿高等研究院的 E. Witten 教授认为时空是注定存在的，而美国哈佛大学 A. Strominger 教授则认为时空或许是一个我们将要放弃的概念。我们能不能认为时间是诱导的？如果时间是诱导的，那么空间也将同样是诱导的。要回答这

个问题就需要回答前面的问题，什么是弦论？这需要做基本概念上的革命。

物理学与环境科学：物理学是否是一个环境科学？描述物理世界的所有参数和法则是否是可以计算的？或者说是否有些是由历史或量子力学事件决定的？

运动学、动力学和初始条件：在传统的物理学中，运动学和动力学是区分开来的。但是在理解弦论和探求时空本质时，运动学和动力学的差别将难以区分，同时量子力学也将变得必不可少和不再神秘。

新物态：是否存在常规实验可以得到非费米流行为的凝聚态物质？

复杂性：描述巨大复杂动力学体系的理论是什么？由于计算机的功能越来越强大，我们希望利用它来预言地球的气候变化、细胞中的化学过程及人类大脑行为。这些体系的混沌特点决定了预言中存在固有极限，但是难以将这些特点从不感兴趣的现象中分离出来。因此，对于理论物理学家来说能否发展一套计算手段来分析这些系统，鉴别它们的特性是一个不小的问题。

量子计算：量子计算机应该是什么样的？在构造量子计算机过程中，主要的障碍是退相干问题，因为外界的扰动会使得量子计算机成为经典计算机。有两个不同的方法可以克服这一问题，一种是通过与外界隔离的办法来尽量减少噪音的扰动，即安静的计算机；另一种是构造不与外界的干扰发生耦合的计算机，即聋哑的计算机。我们是否能真正造出可以实用的量子计算机？

物理学的应用：我们是否知道如何制造出在室温或高于室温的情况下可以应用的超导材料？是否能够利用电子材料（如半导体）制造出室温铁磁体？

理论生物学：什么是生物学的理论？理论物理有助于生物学的研究吗？是否需要新的数学？如何描述生物体呈现出的多时间大尺度动力学体系？

基因学：进化论能否被定量化并且变成可预言的？我们是否可以通过对基因的研究来给出有机体的形状？

意识学：隐藏在记忆和意识后边的潜在的原理是什么？是否可以测量一个婴儿的意识的开始？能否制造具有自由意识、并且具有目的行为能力的机器？

计算物理：物理学中定量计算显得越来越重要，那么计算机是否能代替解析技术？如果是这样，我们该如何调整对物理学家的训练？进而，计算机何时能成为具有创造力的理论物理学家？

物理学的分化：既然物理学有从弦论到生物学多样性，它是否会分化成许多独立的子学科？物理学的分化是否还会继续？我们应该如何面对这种状况？

还原论：我们想当然的认为既然大客体是由小的客体构成的，那么大客体的行为完全由小客体的行为决定，至少原则上是这样。那么比起自然界不能告诉我们她的左手与右手的差别来说，这一点是否是更明显正确？

理论的作用：在物理学和其他科学中理论的正确作用是什么？理论是否仅仅是实验的奴隶，只是通过它预言的实验结果来判断，还是只关注于数学结构的完美而不管是否反映客观世界的真实？在对复杂系统的描述中如何估价物理学家倡导的简洁性和数学结构的优美性等原则？

物理学发展中潜在的危险性：人们可以看到，在未来的 25 年中传统的大物理学工程是不现实的。我们现在应该考虑什么样的新途径，在这一过程中理论学家会起什么样

的作用?

《数学物理学百科全书》包含的内容是研究和回答以上提出的科学问题所必须具备的基础知识。《数学物理学百科全书》导读版的发行，为我国在物理学和数学领域的广大科技工作者和研究生提供了一部全面了解数学物理基础知识和发展前沿，以及核心课题的最具完整性和系统性及权威性的百科全书。《数学物理学百科全书》导读版适合高等院校的广大师生和研究院所的科技人员参考阅读。

在写百科全书导读时，恰逢我国“科学的春天”30 周年纪念和迎来我国改革开放 30 周年。这是一个值得我国科技界庆贺和回顾的 30 年，在“科学技术是第一生产力”的正确论断鼓舞下，以物理学和数学为典型代表的基础研究在我国得到了极大的发展。当前，我国正在全面落实科学发展观，建设创新型国家，提倡自主创新和原始创新。尽管我国的物理学和数学已取得了一系列重要的进展，但作为世界大国和文明古国，还远远没有在这两个最基本的学科领域做出应有的更大的贡献。在 21 世纪的今天，随着我国经济的蓬勃发展和社会的不断进步，面对新的机遇和挑战，广大科技工作者不仅会在物理学和数学这两大基础领域做出原创性工作和历史性贡献，还必将会为整个世界的科技发展、人类文明、社会进步做出中国科学家应有的贡献。

最后，我们要感谢《数学物理学百科全书》导读版编辑委员会的所有成员，他们对导读版的编辑提出许多有用的建议，认真撰写第一卷 8 篇导论性文章的中文译文，对导读版进行仔细审校。特别要感谢科学出版社的编辑孙红梅和霍志国为发行《数学物理学百科全书》导读版所做的一切努力。

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前　言

在过去的几个世纪，我们的物理世界处处充满着神秘。神的力量能带给我们真正的奇迹；水和阳光能使不毛之地变成肥沃的牧场，但它们同样能带来痛苦和灾难。生命之力被认为是对所有生命体负责的特殊力量。凡是它们所在的地方，包括所有星体和其他天体的天堂，都是神的属有领域。

当然，数学是确实存在的。事实上，从某种角度而言，物理学是由精确的数学逻辑所操控的：古希腊人把空间几何结构变成了一种真实的艺术形式。就我所知，古希腊人是“数学物理”的第一个践行者。他们引入了坐标轴的概念，从而把空间几何的所有量都转化为一些简单的数字。今天，这些被称作“物理学的基本定律”。直到很久以后我们才认识到如下事实：**时间**流可以类似地被坐标化，它连同空间一起，同样可用几何方法来解决。于是，有一些疯狂的人对数字的魔力很感兴趣，但是，我们的现实世界似乎确实包含许多超出我们分析能力的地方。

渐渐地，所有这一切都变了。月亮和其他行星的运动好像都满足几何定律。伽利略和牛顿设法去发现这些运动的合乎逻辑的定律，并注意到质量的概念也适用于太空中的物体，就像地球上的苹果和大炮一样；这使得太空更容易被我们所理解。同时人们发现，电子、磁场、光和声音也完全按照数学方程在运转。

然而，所有这一切仅仅是个开始。真正的改变出现在 20 世纪。阿尔伯特·爱因斯坦首先引入了一种全新的思考问题的方式，即通过数学论证和逻辑推理，而非直觉经验。通过只有少数纯数学家才知道的高等的数学知识来研究现实的空间和时间，这对当时的物理学家而言是全新的方法。爱因斯坦本人也是花费了很大的努力来理解这些对今天的数学物理方向的研究生来说是再熟悉不过的联络和曲率的概念，但在当时，这些都是全新的概念。我们不得不佩服爱因斯坦当时有远见的洞察力，他所预见的远不止我们今天在大学教室里所教的那些东西。

狭义和广义相对论仅仅是我们今天用高等的数学方法研究的现代物理学王国的一小角。我们有众所周知的复杂课题，例如，凝聚态物理中的相位转变、超导学、Bose-Einstein 凝聚态、量子 Hall 效应，特别是量子分数 Hall 效应，以及其他很多来自初等粒子物理方面的题目，同时还有来自纤维丛和超重力的重正化群，代数拓扑、超弦理论、Clabi-Yau 空间和其他一些未知方面的问题，所有这些都迫切需要用我们的智慧去理解。

今天我们觉得最不可思议的是，我们的**整个**物理世界好像都被数学方程操控着，并且它们不是草率的和可争议的模型，而是大千世界中各种物质、系统和现象的确实被证明的性质。

数学是否真的适用于整个世界，或仅是世界的一个部分？特征、记号和实体是否是**非**数学地独自存在？我们的直觉、梦想、意识和信仰又如何呢？或许此时大部分人会说，在这些方面我们不需要数学的分析；尽管在这些方面，一些勇敢的社会学家开始试

图用合理的数学方法研究问题。

不，物理世界和数学世界之间存在明显的重要区别。物理世界强调事实的“真相”，无论“真相”是什么，而数学是纯逻辑和纯推理的世界。在物理学中，一个理论是否能被接受是由实验来最后决定的。物理学中的方法论也与数学不同。

一个有趣的例子是超导电性的偶然发现。1911 年，荷兰物理学家 Heike Kamerling Onnes 首先发现液化氦，这是在低于 4.25 K 时实现的。Heike 想要测量水银的传导性，水银是一种低温下会凝固成固体的金属。但测量中出现了一些问题，伏特表根本不显示任何电压。小组中所有富有经验的物理学家都认为出了故障。这种现象在短路电路实验中已经不是第一次出现了，但这一次，他们始终没能找出问题来。有个助手负责保持样品中液化氦的温度，这是一项枯燥乏味的工作，需要一直注视某些细节。然而，在一次测试中他打了个瞌睡，温度上升了，忽然仪器再次出现正常值，研究发现温度是完全可再现的。低于 4.19 K 时，水银的传导性趋于无穷。高于 4.19 K 时是有限的，而这个转变是非常突然的。超导电性由此被发现（D. van Delft，“Heike Kamerling Onnes”，Uitgeverij Bert Bakker，Amsterdam，2005，荷兰）。

这个发现不是用数学的方法。如果助手睡着了，定理也不会被发现，即使例子中确实存在一些神奇的事情。

数学物理这个交叉学科是非常难懂的。百科全书中的某些题目纯粹是物理的。高 T_c 超导电性、破坏水波和磁水动力是完全物理的题目，其中的实验数据比任何高深理论都具有决定性。然而，上同调理论、Donaldson-Witten 理论和 AdS/CFT 对应是纯数学的例子，尽管在这次编辑中这些题目和物理学有着密切的关系。

在编辑中，大量不同作者的短小文章不可避免地被做了适当地变动。在这本百科全书中，理论物理学家和数学家为高等数学物理中的许多重要条目做了简单明了的阐述。所有的文章都包含了供进一步阅读的参考文献。我们盼望这些努力会取得很好的效果。

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（沈一兵　译）

序

数学物理是一门相对较新的独立学科。数学物理国际协会成立于 1976 年。当然，从古时候起数学与物理学就相互影响，但近几十年来，可能因为我们正身在其中，它们出现了巨大的进展，新的结果和观点以令人目眩的节奏诞生，以至于需要有一本百科全书来搜集整理这些知识。

数学物理把数学和物理学这两个大学科的优势集中到一起，它们的关系是共同发展。一方面，它运用数学这一工具把不断增长的精确性和复杂性这些物理概念组织了起来；另一方面，物理学家为数学家们提供了灵感的源泉。两者关系的经典例子是爱因斯坦的相对论，其中微分几何在物理理论的公式化方面起到了实质性的作用，而物理学相继提出的问题推动了微分几何的发展。巧合的是，当我们在为《数学物理学百科全书》写序言时，正值爱因斯坦创造奇迹 100 周年。

再三考虑到写这部《数学物理学百科全书》是一个艰巨的项目。如果不是坚信这是一项很有意义的、受益于社会的项目，而且我们会得到众多的支持，那么我们绝不会接受这个任务。我们确实获得了许多支持，包括建议、鼓励和有实用性的帮助，这些支持来自编辑顾问委员会成员和我们的作者，还有其他慷慨地抽时间帮我们完善这本百科全书的人。

数学物理是一门较新的学科，它还没有被清晰地刻画，不同的人对它有不同的理解。在我们选择的题目中，一部分遵循了近期数学物理国际大会的纲要，但主要参照编辑顾问委员会和作者的提议。由于时间和空间的限制，以及我们自身的水平所限，更改了某些冗长的题目，但我们尽量收录了我们认为是核心的课题，尽量覆盖更多的最活跃的领域。

由于我们的课题是跨学科的，这部百科全书应当有某些特殊的特色。比如，同一数学理论应用到不同的物理问题时，会有不同的侧重点和处理方法。同样，相同的物理问题可以运用不同数学领域的方法。这就是为什么我们把百科全书分成了两个广阔的部分：物理学课题和相关的数学课题。每一部分的文章允许与其他部分有相当的重复，许多文章会出现在多个标题下，不过它们都被精心制作的对照表联接起来。我们认为，这会给课题的整体性做出更好的描述，为来自广泛的相关领域的研究者提供更好的服务。

百科全书主要针对有经验的研究者，不过也会对初学的研究生有用。对于后者，我们收录了 8 篇初等的导论性文章，以便于参考，其中数学文章是针对物理研究生的，物理文章是针对数学研究生的，这些文章可以作为他们在阅读主体文章前的准备，而不需要查阅其他资料。事实上，这些文章可以作为高年级研究生课程的基础，因为据我们所知，某些作者已经这样做了。

除了印刷版外，百科全书的网络在线版正在计划中，以便目录和文章本身内容及时得到更新。对于飞速发展的这一领域而言，这可能是一个必要的准备。

这个项目进行了 4 年多。对于它的完成，我们首先要感谢编辑顾问委员会的所有成

员，他们为我们提建议，始终帮助和鼓励我们；也要感谢所有的作者，他们慷慨地献出宝贵的时间来写这些文章，并提出了许多有用的建议。在与他们的合作中我们学到了许多东西，并与其中一些作者有过美好的接触。特别要感谢 Arthur Greenspoon，他的专业技术是必不可少的。

这个项目开始于 Academic Press，后来由 Elsevier 接手。感谢他们的热情的工作人员，把过渡工作做得天衣无缝，在工作上也给了我们巨大的帮助：Carey Chapman 和 Anne Guillaume 掌管着整个项目，自始至终和我们一起工作；Edward Taylor 负责审稿；Martin Ruck 负责具体事务，特别要提到的是，从没听说过有某封电子邮件丢失。

最后，要对相当一部分作者慷慨地把他们的酬劳捐赠给欧洲数学会的发展中国家委员会表示由衷的感谢，感谢他们为发展中国家所做的一切。

Jean- Pierre Françoise
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（沈一兵　译）

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FOREWORD

In bygone centuries, our physical world appeared to be filled to the brim with mysteries. Divine powers could provide for genuine miracles; water and sunlight could turn arid land into fertile pastures, but the same powers could lead to miseries and disasters. The force of life, the *vis vitalis*, was assumed to be the special agent responsible for all living things. The heavens, whatever they were for, contained stars and other heavenly bodies that were the exclusive domain of the Gods.

Mathematics did exist, of course. Indeed, there was one aspect of our physical world that was recognised to be controlled by precise, mathematical logic: the geometric structure of space, elaborated to become a genuine form of art by the ancient Greeks. From my perspective, the Greeks were the first practitioners of 'mathematical physics', when they discovered that all geometric features of space could be reduced to a small number of axioms. Today, these would be called 'fundamental laws of physics'. The fact that the flow of *time* could be addressed with similar exactitude, and that it could be handled geometrically together with space, was only recognised much later. And, yes, there were a few crazy people who were interested in the magic of numbers, but the real world around us seemed to contain so much more that was way beyond our capacities of analysis.

Gradually, all this changed. The Moon and the planets appeared to follow geometrical laws. Galilei and Newton managed to identify their logical rules of motion, and by noting that the concept of mass could be applied to things in the sky just like apples and cannon balls on Earth, they made the sky a little bit more accessible to us. Electricity, magnetism, light and sound were also found to behave in complete accordance with mathematical equations.

Yet all of this was just a beginning. The real changes came with the twentieth century. A completely new way of thinking, by emphasizing mathematical, logical analysis rather than empirical evidence, was pioneered by Albert Einstein. Applying advanced mathematical concepts, only known to a few pure mathematicians, to notions as mundane as space and time, was new to the physicists of his time. Einstein himself had a hard time struggling through the logic of connections and curvatures, notions that were totally new to him, but are only too familiar to students of mathematical physics today. Indeed, there is no better testimony of Einstein's deep insights at that time, than the fact that we now teach these things regularly in our university classrooms.

Special and general relativity are only small corners of the realm of modern physics that is presently being studied using advanced mathematical methods. We have notoriously complex subjects such as phase transitions in condensed matter physics, superconductivity, Bose–Einstein condensation, the quantum Hall effect, particularly the fractional quantum Hall effect, and numerous topics from elementary particle physics, ranging from fibre bundles and renormalization groups to supergravity, algebraic topology, superstring theory, Calabi–Yau spaces and what not, all of which require the utmost of our mental skills to comprehend them.

The most bewildering observation that we make today is that it seems that our *entire* physical world appears to be controlled by mathematical equations, and these are not just sloppy and debatable models, but precisely documented properties of materials, of systems, and of phenomena in all echelons of our universe.

Does this really apply to our entire world, or only to parts of it? Do features, notions, entities exist that are emphatically *not* mathematical? What about intuition, or dreams, and what about consciousness? What about religion? Here, most of us would say, one should not even try to apply mathematical analysis, although even here, some brave social scientists are making attempts at coordinating rational approaches.

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No, there are clear and important differences between the physical world and the mathematical world. Where the physical world stands out is the fact that it refers to 'reality', whatever 'reality' is. Mathematics is the world of pure logic and pure reasoning. In physics, it is the experimental evidence that ultimately decides whether a theory is acceptable or not. Also, the methodology in physics is different.

A beautiful example is the serendipitous discovery of superconductivity. In 1911, the Dutch physicist Heike Kamerlingh Onnes was the first to achieve the liquefaction of helium, for which a temperature below 4.25 K had to be realized. Heike decided to measure the specific conductivity of mercury, a metal that is frozen solid at such low temperatures. But something appeared to go wrong during the measurements, since the volt meter did not show any voltage at all. All experienced physicists in the team assumed that they were dealing with a malfunction. It would not have been the first time for a short circuit to occur in the electrical equipment, but, this time, in spite of several efforts, they failed to locate it. One of the assistants was responsible for keeping the temperature of the sample well within that of liquid helium, a dull job, requiring nothing else than continuously watching some dials. During one of the many tests, however, he dozed off. The temperature rose, and suddenly the measurements showed the normal values again. It then occurred to the investigators that the effect and its temperature dependence were completely reproducible. Below 4.19 degrees Kelvin the conductivity of mercury appeared to be strictly infinite. Above that temperature, it is finite, and the transition is a very sudden one. Superconductivity was discovered (D. van Delft, "Heike Kamerling Onnes", Uitgeverij Bert Bakker, Amsterdam, 2005 (in Dutch)).

This is not the way mathematical discoveries are made. Theorems are not produced by assistants falling asleep, even if examples do exist of incidents involving some miraculous fortune.

The hybrid science of mathematical physics is a very curious one. Some of the topics in this Encyclopedia are undoubtedly physical. High T_c superconductivity, breaking water waves, and magneto-hydrodynamics, are definitely topics of physics where experimental data are considered more decisive than any high-brow theory. Cohomology theory, Donaldson–Witten theory, and AdS/CFT correspondence, however, are examples of purely mathematical exercises, even if these subjects, like all of the others in this compilation, are strongly inspired by, and related to, questions posed in physics.

It is inevitable, in a compilation of a large number of short articles with many different authors, to see quite a bit of variation in style and level. In this Encyclopedia, theoretical physicists as well as mathematicians together made a huge effort to present in a concise and understandable manner their vision on numerous important issues in advanced mathematical physics. All include references for further reading. We hope and expect that these efforts will serve a good purpose.

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PREFACE

Mathematical Physics as a distinct discipline is relatively new. The International Association of Mathematical Physics was founded only in 1976. The interaction between physics and mathematics has, of course, existed since ancient times, but the recent decades, perhaps partly because we are living through them, appear to have witnessed tremendous progress, yielding new results and insights at a dizzying pace, so much so that an encyclopedia seems now needed to collate the gathered knowledge.

Mathematical Physics brings together the two great disciplines of Mathematics and Physics to the benefit of both, the relationship between them being symbiotic. On the one hand, it uses mathematics as a tool to organize physical ideas of increasing precision and complexity, and on the other it draws on the questions that physicists pose as a source of inspiration to mathematicians. A classical example of this relationship exists in Einstein's theory of relativity, where differential geometry played an essential role in the formulation of the physical theory while the problems raised by the ensuing physics have in turn boosted the development of differential geometry. It is indeed a happy coincidence that we are writing now a preface to an encyclopedia of mathematical physics in the centenary of Einstein's annus mirabilis.

The project of putting together an encyclopedia of mathematical physics looked, and still looks, to us a formidable enterprise. We would never have had the courage to undertake such a task if we did not believe, first, that it is worthwhile and of benefit to the community, and second, that we would get the much-needed support from our colleagues. And this support we did get, in the form of advice, encouragement, and practical help too, from members of our Editorial Advisory Board, from our authors, and from others as well, who have given unstintingly so much of their time to help us shape this Encyclopedia.

Mathematical Physics being a relatively new subject, it is not yet clearly delineated and could mean different things to different people. In our choice of topics, we were guided in part by the programs of recent International Congresses on Mathematical Physics, but mainly by the advice from our Editorial Advisory Board and from our authors. The limitations of space and time, as well as our own limitations, necessitated the omission of certain topics, but we have tried to include all that we believe to be core subjects and to cover as much as possible the most active areas.

Our subject being interdisciplinary, we think it appropriate that the Encyclopedia should have certain special features. Applications of the same mathematical theory, for instance, to different problems in physics will have different emphasis and treatment. By the same token, the same problem in physics can draw upon resources from different mathematical fields. This is why we divide the Encyclopedia into two broad sections: physics subjects and related mathematical subjects. Articles in either section are deliberately allowed a fair amount of overlap with one another and many articles will appear under more than one heading, but all are linked together by elaborate cross referencing. We think this gives a better picture of the subject as a whole and will serve better a community of researchers from widely scattered yet related fields.

The Encyclopedia is intended primarily for experienced researchers but should be of use also to beginning graduate students. For the latter category of readers, we have included eight elementary introductory articles for easy reference, with those on mathematics aimed at physics graduates and those on physics aimed at mathematics graduates, so that these articles can serve as their first port of call to enable them to embark on any of the main articles without the need to consult other material beforehand. In fact, we think these articles may even form the

foundation of advanced undergraduate courses, as we know that some authors have already made such use of them.

In addition to the printed version, an on-line version of the Encyclopedia is planned, which will allow both the contents and the articles themselves to be updated if and when the occasion arises. This is probably a necessary provision in such a rapidly advancing field.

This project was some four years in the making. Our foremost thanks at its completion go to the members of our Editorial Advisory Board, who have advised, helped and encouraged us all along, and to all our authors who have so generously devoted so much of their time to writing these articles and given us much useful advice as well. We ourselves have learnt a lot from these colleagues, and made some wonderful contacts with some among them. Special thanks are due also to Arthur Greenspoon whose technical expertise was indispensable.

The project was started with Academic Press, which was later taken over by Elsevier. We thank warmly members of their staff who have made this transition admirably seamless and gone on to assist us greatly in our task: both Carey Chapman and Anne Guillaume, who were in charge of the whole project and have been with us since the beginning, and Edward Taylor responsible for the copy-editing. And Martin Ruck, who manages to keep an overwhelming amount of details constantly at his fingertips, and who is never known to have lost a single email, deserves a very special mention.

As a postscript, we would like to express our gratitude to the very large number of authors who generously agreed to donate their honorariums to support the Committee for Developing Countries of the European Mathematical Society in their work to help our less fortunate colleagues in the developing world.

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导论:经典力学

基本原理

经典力学是一门关于点粒子运动的理论。设若粒子在笛卡儿惯性坐标系中的位置为 $\boldsymbol{X}=(x_1,\cdots,x_n)$,则运动由粒子的质量$(m_1,\cdots,m_n)$,$m_j>0$,以及相互作用势 $V(x_1,\cdots,x_n)$通过方程

$$m_i\ddot{x}_i=-\partial_{x_i}V(x_1,\cdots,x_n),\qquad i=1,\cdots,n \tag{1}$$

所决定,这里 $x_i=(x_{i1},\cdots,x_{id})$为第 i 个粒子的的坐标,∂_{x_i} 为梯度$(\partial_{x_1},\cdots,\partial_{x_d})$; d 是空间的维度(一般地,$d=3$)。势能函数假设是“光滑”的,即除了在可能的两粒子位置重合的情形下它是解析的。为了包括引力势,或在处理带电粒子所涉及的库仑势,上述例外是必需的。一个基本结果是,如果 V 是有下界的,则给定了初始条件 $\boldsymbol{X}_0=\boldsymbol{X}(0),\dot{\boldsymbol{X}}_0=\dot{\boldsymbol{X}}(0)$,方程[1]有惟一的全局解 $t\mapsto\boldsymbol{X}(t),t\in(-\infty,\infty)$;否则,当且仅当解在有限时间内到达无穷远点或落入奇点(即两个或多个粒子占据同一点那样的构形,也即发生了碰撞)时,解可以不是全局的。

在方程[1]中,$-\partial_{x_i}V(x_1,\cdots,x_n)$是作用在粒子上的力。更一般形式的力也会经常遇到,比如依赖于速度的摩擦力。我们这里不考虑摩擦力,因为其本质上是关于微观现象的唯象模型(即使在宏观的层面上摩擦力也是不完全的模型,它们应该和伴随着的热产生现象一同考虑),原则上是可以用保守力解释的。另一类有趣的、不对应于一个势能的力是类似科里奥利力(只出现在非惯性系中)和洛伦兹力(电磁学)那样的依赖于速度的力,它们很容易在力学的哈密顿表述的框架中处理,参见附录二。

与方程[1]等价的作用量原理可表述为:满足方程[1]的、在时间间隔$[t_1,t_2]$内从点 $\boldsymbol{X}^1=\boldsymbol{X}_0(t_1)$到点 $\boldsymbol{X}^2=\boldsymbol{X}_0(t_2)$ 的运动 $t\mapsto\boldsymbol{X}_0(t)$使作用量

$$\mathcal{A}(\{\boldsymbol{X}\})=\int_{t_1}^{t_2}\Big(\sum_{i=1}^{n}\frac{1}{2}m_i\dot{\boldsymbol{X}}_i(t)^2-V(\boldsymbol{X}(t))\Big)\mathrm{d}t \tag{2}$$

在 $\mathcal{M}_{t_1,t_2}(\boldsymbol{X}^1,\boldsymbol{X}^2)$中平稳,而 $\mathcal{M}_{t_1,t_2}(\boldsymbol{X}^1,\boldsymbol{X}^2)$,定义为在 $t\in[t_1,t_2]$间隔内从点 $\boldsymbol{X}^1$ 到点 $\boldsymbol{X}^2$ 的光滑(即解析的)“运动” $t\mapsto\boldsymbol{X}(t)$组成的集合。

函数

$$\mathcal{L}(\boldsymbol{Y},\boldsymbol{X})=\frac{1}{2}\sum_{i=1}^{n}m_iy_i^2-V(\boldsymbol{X})\overset{\text{def}}{=}K(\boldsymbol{Y})-V(\boldsymbol{X})$$

$$\boldsymbol{Y}=(y_1,\cdots,y_n)$$

称为拉格朗日函数,而作用量可写成

$$\int_{t_1}^{t_2}\mathcal{L}(\dot{\boldsymbol{X}}(t),\boldsymbol{X}(t))\mathrm{d}t$$

量 $K(\dot{\boldsymbol{X}}(t))$是动能。满足方程[1]的运动保持能量不变,即

$$K(\dot{\boldsymbol{X}}(t))+V(X(t))=E=\text{常数} \tag{3}$$

因此,作用量原理可以直观上认为是说:运动在保持能量——动能与势能之和——守恒的同时尽可能均等地分配(在时间平均的意义上)对能量的贡献。

在 V 是平移对称的特例中,运动保持线性动量 $Q\overset{\text{def}}{=}\sum_i m_i\dot{x}_i$ 不变;而如果 V 是关于原点 O 转动不变的,则运动保持角动量 $M\overset{\text{def}}{=}\sum_i m_i x_i\wedge\dot{x}$ 不变,这里 $\wedge$ 表示 R^d 空间中的矢量积,即为张量 $(\boldsymbol{a}\wedge\boldsymbol{b})_{ij}=a_ib_j-b_ia_j$, $i,j=1,\cdots,d$。如果维度 $d=3$, $\boldsymbol{a}\wedge\boldsymbol{b}$ 自然可以认为它是矢量[①]。更一般地,对任何拉格朗日量的连续变换群都对应着守恒量,这一点由 **Noether 定理所表述**。

空间 R^{dn} 中的标量积可方便地由常规的 R^d 空间中的标量积 $\boldsymbol{a}\cdot\boldsymbol{b}=\sum_{j=1}^{d}a_jb_j$ 通过 $(\boldsymbol{v},\boldsymbol{w})=\sum_{i=1}^{n}m_i\boldsymbol{v}_i\cdot\boldsymbol{w}_i$ 来定义,这样动能和线元 $\mathrm{d}s$ 可分别写为 $K(\dot{\boldsymbol{X}})=\frac{1}{2}(\dot{\boldsymbol{X}},\dot{\boldsymbol{X}})$ 和 $\mathrm{d}s^2=\sum_{i=1}^{n}m_i\mathrm{d}x_i^2$。因此,由后一个标量积生成的度量被称为**动能度量**。

动能度量的意义体现在 Maupertuis **原理**(等价于方程[1])中,它能够把 R^d 空间中由能量为 E、从点 $\boldsymbol{X}^1$ 到点 $\boldsymbol{X}^2$ 的运动所划过的轨迹识别出来。把运动轨迹参数化为 $\tau\mapsto\boldsymbol{X}(\tau)$,参数 τ 在[0,1]区间内变化,使得线元可表示为 $\mathrm{d}s^2=(\partial_\tau\boldsymbol{X},\partial_\tau\boldsymbol{X})\mathrm{d}\tau^2$,则该原理宣称在所有的解析曲线 $\xi\in\mathcal{M}_{0,1}(\boldsymbol{X}^1,\boldsymbol{X}^2)$ 中,能量为 E、从点 $\boldsymbol{X}^1$ 到点 $\boldsymbol{X}^2$ 的运动所划过的轨迹平稳化,函数

$$L(\xi)=\int_\xi\sqrt{E-V(\xi(s))}\,\mathrm{d}s \qquad [4]$$

这使得能量为 E 的方程[1]的解在 R^{nd} 空间中划过的轨迹等同于度量 $\mathrm{d}m^2\overset{\text{def}}{=}(E-V(\boldsymbol{X}))\cdot\mathrm{d}s^2$ 下的测地线。

更详细的内容请参阅 Laudau,Lifshitz(1976) 和 Gallavotti(1983)。

约束

粒子经常会被置于约束之下,被限制在曲面 $M\subset R^{nd}$ 上运动,即 $\boldsymbol{X}(t)$ 只能是流形 M 上的点。典型的例子是刚体运动,物体所受的力应保持粒子间的距离 $|\boldsymbol{x}_i-\boldsymbol{x}_j|=\rho_{ij}$ 不变,ρ_{ij} 是一个不依赖于时间的正的常量。实际上,所有造成约束的力,称为约束反作用,都是依赖于速度的,因而不是此处考虑的这类保守力,见方程[1]。因此,从只允许保守力的基本观点来看,约束系统应该被看作是置于(近似地意味着约束的)保守力之下系统的理想化。

一般地,ℓ 维的流形 M 没有整体的坐标系,但可以用在开球 $B_{\boldsymbol{X}^0}:\boldsymbol{X}=\boldsymbol{X}(q_1,\cdots,q_\ell,q_{\ell+1},\cdots,q_N)$ 中变化的 $N=nd$ 个坐标 $q=(q_1,\cdots,q_\ell,q_{\ell+1},\cdots,q_N)$ 来描述 $\boldsymbol{X}^0\in M$ 邻域内的点。q 坐标可很好地选择来适应曲面 M 和动能度量,即对于 M 上的点有 $q_{\ell+1}=\cdots=q_N=0$(这就是"适应"的含义);自点 $\boldsymbol{X}^0\in M$ 向外的无穷小位移 $(0,\cdots,0,\mathrm{d}\varepsilon_{\ell+1},\cdots,\mathrm{d}\varepsilon_N)$ 正交于 M(在动测度量下)且其长度不依赖点 $\boldsymbol{X}^0$ 在 M 上的位置(这是"很好地适应于"动测度量的意思)。

当势能 V 具有

$$V(\boldsymbol{X})=V_a(\boldsymbol{X})+\lambda W(\boldsymbol{X}) \qquad [5]$$

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① 这个说法不对。请读者参阅 David Hestenes 著 New Fundamentals of Classical Mechanics——译者注。

的形式时,其中 W 是在流形 M 上取极小值——比如零——的光滑函数,而 V_a 是另一光滑的势能函数,则 M 上的约束运动就发生了。式[5]中的参数因子 $\lambda>0$ 被称为约束刚度。

特别有趣的情况发生在 W 的水准面同曲面 M 平行时,这里平行的确切含义是在任何很好地适应于动能度量的坐标系里,对所有的点 $\boldsymbol{X}\in M$,矩阵 $\partial^2_{q_iq_j}W(\boldsymbol{X})$,$i,j>\ell$,是正定的且不依赖于 $\boldsymbol{X}$。具有上述性质的 W 可以称为近似理想的约束反作用。实际上,可以证明,给定初始值 $\boldsymbol{X}^0\in M$ 和与 M 相切的速度 $\dot{\boldsymbol{X}}_0$,即在某局域坐标系中给定初始值 $(\boldsymbol{q}_0,0)$ 和 $(\dot{\boldsymbol{q}}_0,0)$,$\boldsymbol{q}_0=(q_{01},\cdots,q_{0\ell})$,$\dot{\boldsymbol{q}}_0=(\dot{q}_{01},\cdots,\dot{q}_{0\ell})$,则由方程[1]在式[5]给出的势能 V 下所引起的运动为 $t\mapsto\boldsymbol{X}_\lambda(t)$,且

(1) 当 $\lambda\to\infty$ 时,它趋于运动 $t\to\boldsymbol{X}_\infty(t)$;

(2) 只要 $X_\infty(t)$,如对于 $0\leqslant t\leqslant t_1$,还停留在初始值附近,则它可以用上述局域坐标系描述,它的坐标有形式 $t\to(\boldsymbol{q}(t),0)=(q_1(t),\cdots,q_\ell(t),0,\cdots,0)$:即运动被约束在 M 上;

(3) 曲线 $t\to\boldsymbol{X}_\infty(t)$,$t\in[0,t_1]$,作为 M 上连接 $\boldsymbol{X}^0$ 和 $\boldsymbol{X}_\infty(t_1)$ 的解析曲线所构成的空间 $\mathcal{M}_{0,t_1}(\boldsymbol{X}^0,\boldsymbol{X}_\infty(t))$ 的一个元素,使得作用量

$$A(\boldsymbol{X})=\int_0^{t_1}(K(\dot{\boldsymbol{X}}(t))-V_a(\boldsymbol{X}(t)))\,\mathrm{d}t \qquad [6]$$

是稳定的。

后一个性质可以"内禀"的方式表述,即只涉及曲面 M,通过把度量 $\mathrm{d}s^2$ 限制到在点 $\boldsymbol{X}=(q_0,0,\cdots,0)\in M$ 处与 M 相切的线元 $\mathrm{d}s=(\mathrm{d}q_1,\cdots,\mathrm{d}q_\ell,0,\cdots,0)$ 上,我们有 $\mathrm{d}s^2=\sum_{i,j}^{1,\ell}g_{ij}(q)\times\mathrm{d}q_i\mathrm{d}q_j$,其中对称的、正定的 $\ell\times\ell$ 矩阵 q 称为 M 上由动能诱导的**度量**。作用量[6]可写为

$$A(\boldsymbol{q})=\int_0^{t_1}\left(\frac{1}{2}\sum_{i,j}^{1,\ell}g_{ij}(\boldsymbol{q}(t))\dot{q}_i(t)\dot{\boldsymbol{q}}_j(t)-\overline{V_a}(\boldsymbol{q}(t))\right)\mathrm{d}t \qquad [7]$$

其中 $\overline{V_a}(\boldsymbol{q})\overset{\mathrm{def}}{=}V_a(\boldsymbol{X}(q_1,\cdots,q_\ell,0,\cdots,0))$,而函数

$$\mathcal{L}(\boldsymbol{\eta},\boldsymbol{q})\overset{\mathrm{def}}{=}\frac{1}{2}\sum_{i,j}^{1,\ell}g_{ij}(\boldsymbol{q})\eta_i\eta_j-\overline{V_a}(\boldsymbol{q})\equiv\frac{1}{2}g(\boldsymbol{q})\boldsymbol{\eta}\cdot\boldsymbol{\eta}-\overline{V_a}(\boldsymbol{q}) \qquad [8]$$

被称为系统的约束拉格朗日量。

约束运动保持能量 $E=\frac{1}{2}(g(\boldsymbol{q})\dot{\boldsymbol{q}},\dot{\boldsymbol{q}})+\overline{V_a}(\boldsymbol{q})$ 不变,这是一个重要的性质;请参阅下一节。

能量为 E 的约束运动 $\boldsymbol{X}_\infty(t)$ 满足 Maupertuis 原理,即运动在 M 上划过的曲线在所有的在 M 上连接固定的 $\boldsymbol{X}^1$ 和 $\boldsymbol{X}^2$ 的(光滑)曲线中使得

$$L(\boldsymbol{\xi})=\int_\xi\sqrt{E-V_a(\boldsymbol{\xi}(s))}\,\mathrm{d}s \qquad [9]$$

为平稳的。当 $\ell=n$ 时的特例就是在势场 $V(\boldsymbol{X})$ 中无约束运动的 Maupertuis 原理。因为对初始值的完备描述需要 2ℓ 个坐标 $\boldsymbol{q}(0)$ 和 $\dot{\boldsymbol{q}}(0)$,ℓ 一般被称为自由度。

如果 W 在流形 M 上为极小但 W 的水准面同 M 平行的条件不能得到满足,就是说如果 W 不是近似理想的约束反作用,则极限运动 $\boldsymbol{X}_\infty(t)$ 同样会在 M 上发生,只是一般地它不再能满足上述的变分原理。因此,作为势场[5]——其中 W 在 M 上取极小值且其水准面同 W 平行——中的运动之极限($\lambda\to\infty$)的运动就被称为理想约束运动或被理想约束限制在 M 表

面上的运动。

现举一例。假设 $W(\boldsymbol{X})=\sum_{i,j\in P}w_{ij}(|\boldsymbol{x}_i-\boldsymbol{x}_j|)$，其中 $w_{ij}(|\boldsymbol{\xi}|)\geqslant 0$，是一解析函数，且仅当 $|\boldsymbol{\xi}|=\rho_{ij}$（对于 i,j 在 P 的特定集合中和一些给定的距离 ρ_{ij}）时函数为零（比如 $W_{ij}(\boldsymbol{\xi})=(\boldsymbol{\xi}^2-\rho_{ij}{}^2)^2\gamma,\gamma>0$），则可证 W 满足上述的条件，因此其上的约束运动 $X_\infty(t)$ 满足同式[7]和式[9]相联系的变分原理。换句话说，上述实现一个相当一般刚性约束的自然方式是理想的。

关于约束反作用之物理意义的现代观点如下：考察惯性笛卡儿坐标系中的运动，系统可看作置于势能 $V_a(\boldsymbol{X})$ 所对应的外力和可表为 $R_i=m_i\ddot{\boldsymbol{x}}_i+\partial_{x_i}V_a(\boldsymbol{X})$ 的约束力之下，后者反映的是势能 $\lambda W(\boldsymbol{X})$ 在无穷大刚性极限 $\lambda\to\infty$ 下的作用力。

实际应用中，约束的作用有时可看作是理想的：运动将证实前述的变分原理，而 $\boldsymbol{R}$ 可由 $m_i\ddot{\boldsymbol{x}}_i$ 和主动力 $-\partial_{x_i}V_a(\boldsymbol{X})$ 之差计算出来。对于动力学问题，特别是有关工程问题，一件重要的也是非常困难的事情就是判断是否一个粒子系统是置于理想约束之下的，这对机械的设计制造是至关重要的。它可以简化反作用和材料疲劳的计算，而误判会在稳定性与安全性方面造成严重的后果。对于静力学问题，困难要小一点：假设约束反作用是理想的通常会导致对平衡稳定性条件的过高估计。因此，把作用量原理运用于静力学问题，这时它构成所谓的**虚功**原理，一般地会造成经济问题而非关安全性。这一点早在牛顿力学出现之前人们就注意到了。

更多的细节请参阅 Arnol′d(1989) 和 Gallavotti(1983)。

运动方程的拉格朗日和哈密顿形式

作用量 $A(q)$（见式[7]和式[8]）的平稳性条件可用拉格朗日量 $\mathcal{L}(\boldsymbol{\eta},\boldsymbol{\xi})$（见[8]）表述为

$$\frac{\mathrm{d}}{\mathrm{d}t}\partial_{\eta_i}\mathcal{L}(\dot{\boldsymbol{q}}(t),\boldsymbol{q}(t))=\partial_{\xi_i}\mathcal{L}(\dot{\boldsymbol{q}}(t),\boldsymbol{q}(t)),\ i=1,\cdots,\ell \qquad [10]$$

这是一个二阶微分方程，称为拉格朗日运动方程。它可以写成一个标准形式：为此采用对重复指标求和的惯例，引入“广义动量”

$$p_i\overset{\text{def}}{=}g(\boldsymbol{q})_{ij}\dot{q}_j,\ i=1,\cdots,\ell \qquad [11]$$

由于 $g(\boldsymbol{q})>0$，运动 $t\to\boldsymbol{q}(t)$ 和相应的速度 $t\to\dot{\boldsymbol{q}}(t)$ 可等价地描述为 $t\to(\boldsymbol{q}(t),\boldsymbol{p}(t))$，运动方程[10]就变成了一阶方程

$$\dot{q}_i=\partial_{p_i}\mathcal{H}(\boldsymbol{p},\boldsymbol{q}),\dot{\boldsymbol{p}}_i=-\partial_{q_i}\mathcal{H}(\boldsymbol{p},\boldsymbol{q}) \qquad [12]$$

这里函数 $\mathcal{H}$ 称为系统的哈密顿量，定义为

$$\mathcal{H}(\boldsymbol{p},\boldsymbol{q})\overset{\text{def}}{=}\frac{1}{2}(g(\boldsymbol{q})^{-1}\boldsymbol{p},\boldsymbol{p})+\overline{V_a}(\boldsymbol{q}) \qquad [13]$$

方程[12]可看作是相空间的点 $(\boldsymbol{p},\boldsymbol{q})$ 的运动方程，称为哈密顿方程。一般地，$\boldsymbol{q}$ 是 M 上的局域坐标，而运动通过给出 $\boldsymbol{q},\dot{\boldsymbol{q}}$ 或 $\boldsymbol{q},\boldsymbol{p}$ 加以标记。

为找寻对运动不依赖于坐标系的描述，考虑变量对 $\boldsymbol{X},\boldsymbol{Y},\boldsymbol{X}\in M$，而 $\boldsymbol{Y}$ 是在 $\boldsymbol{X}$ 点同 M 相切的矢量 $\boldsymbol{Y}\in T_X$。对 $(\boldsymbol{Y},\boldsymbol{X})$ 的集合记为 $T(M)=\bigcup_{\boldsymbol{X}\in M}(T_{\boldsymbol{X}}\times\{X\})$，局域坐标中的运动 $t\to(\boldsymbol{X}(t),\dot{\boldsymbol{X}}(t))\in T(M)$ 表示为 $(\dot{\boldsymbol{q}}(t),\boldsymbol{q}(t))$。此空间 $T(M)$ 可称为拉格朗日运动方程具有维度 2ℓ 的初始值空间（有时也称为 M 的“切丛”）。

类似的,哈密顿运动方程的初始值空间记为 $T^*(M)$,由对 $\boldsymbol{X},\boldsymbol{P}$ 构成,$\boldsymbol{X}\in M,\boldsymbol{P}=g(\boldsymbol{X})\boldsymbol{Y}$,其中 $\boldsymbol{Y}$ 是在点 $\boldsymbol{X}$ 处与 M 相切的矢量。空间 $T^*(M)$称为系统的相空间,维度也是 $2l$(有时也称为 M 的"余切丛")。

方程[12] 的直接结果是 $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(\boldsymbol{p}(t),\boldsymbol{q}(t))\equiv 0$,它表明 $\mathcal{H}(\boldsymbol{p}(t),\boldsymbol{q}(t))$是关于[12]解的常量。注意到 $\mathcal{H}(\boldsymbol{p},\boldsymbol{q})=\frac{1}{2}(g(q)^{-1}\boldsymbol{p},\boldsymbol{p})+\overline{V_a}(\boldsymbol{q})$是动能和势能之和,则 H 关于解的守恒意味着能量在理想约束下是守恒的。

用 S_t 表示方程[12]的解在相空间变量$(\boldsymbol{p},\boldsymbol{q})$上产生的流,即 $t\to S_t(\boldsymbol{p},\boldsymbol{q})\equiv(\boldsymbol{p}(t),\boldsymbol{q}(t))$表示方程[12]关于初始值$(\boldsymbol{p},\boldsymbol{q})$的解,则相空间一个(可测的)集合 Δ 随时间演化成体积不变的新集合 $S_t\Delta$:这一点是显然的,因为哈密顿方程[12]表明其散度为零("刘维尔定理")。

哈密顿方程也满足变分原理,称为哈密顿作用量原理,即若 $\mathcal{M}_{t_1,t_2}((\boldsymbol{p}_1,\boldsymbol{q}_1),(\boldsymbol{p}_2,\boldsymbol{q}_2);M)$表示在时间间隔$[t_1,t_2]$内从$(\boldsymbol{p}_1,\boldsymbol{q}_1)$到$(\boldsymbol{p}_2,\boldsymbol{q}_2)$的解析函数 $\boldsymbol{\varphi}:t\to(\boldsymbol{\pi}(t),\boldsymbol{\kappa}(t))$组成的空间,则$\boldsymbol{\varphi}_0(t)=(\boldsymbol{p}(t),\boldsymbol{q}(t))$满足方程[12]的条件可等价地表示为要求函数

$$\mathcal{A}_{\mathcal{H}}(\boldsymbol{\varphi})\overset{\mathrm{def}}{=}\int_{t_1}^{t_2}(\boldsymbol{\pi}(t)\cdot\dot{\boldsymbol{k}}(t)-\mathcal{H}(\boldsymbol{\pi}(t),\boldsymbol{k}(t)))\,\mathrm{d}t \qquad [14]$$

关于 $\boldsymbol{\varphi}=\varphi_0$ 是平稳的:实际上,方程[12]就是 $\mathcal{M}_{t_0,t_1}((\boldsymbol{p}_1,\boldsymbol{q}_1),(\boldsymbol{p}_2,\boldsymbol{q}_2);M)$上哈密顿作用量[14]的稳定性条件。因为 $\boldsymbol{\pi}(t)$的导数未出现在方程[14]中,稳定性甚至可以在更大的、关于从 $\boldsymbol{q}_1$ 到 $\boldsymbol{q}_2$ 运动但对动量 $\boldsymbol{p}_1,\boldsymbol{p}_2$ 没有限制(因此也就不能独立于 $\boldsymbol{q}_1,\boldsymbol{q}_2$ 预先确定)的 $\boldsymbol{\varphi}:t\to(\boldsymbol{\pi}(t),\boldsymbol{\kappa}(t))$运动组成的空间 $\mathcal{M}_{t_1,t_2}(\boldsymbol{q}_1,\boldsymbol{q}_2;M)$上实现。如果预先给定的 $\boldsymbol{p}_1,\boldsymbol{q}_1,\boldsymbol{p}_2,\boldsymbol{q}_2$ 和运动方程不相容(比如 $H(\boldsymbol{p}_1,\boldsymbol{q}_1)\neq H(\boldsymbol{p}_2,\boldsymbol{q}_2)$)[①],则作用量泛函在 $\mathcal{M}_{t_1,t_2}((\boldsymbol{p}_1,\boldsymbol{q}_1),(\boldsymbol{p}_2,\boldsymbol{q}_2);M)$内没有平衡轨迹。

欲知更多的细节,读者可参阅 Landau, Lifshitz(1976), Arnol'd(1989) 和 Gallavotti(1983)。

相空间坐标的正则变换

运动方程的哈密顿形式[13]对许多问题非常有用,因此,有必要指出它在一类特殊的坐标变换——称为正则变换——下是不变的。

考虑相空间坐标系的一个局域变换,即在自由度为 l 的哈密顿系统相空间的开集 U 和一个 $2l$ 维空间的开集 U'之间的一个光滑的且光滑得可逆的映射 $C(\boldsymbol{\pi},\boldsymbol{\kappa})=(\boldsymbol{\pi}',\boldsymbol{\kappa}')$。如果对于任何如[12]那样方程的解 $t\to(\boldsymbol{\pi}(t),\boldsymbol{\kappa}(t))$,及任何定义在 U 上相应的哈密顿量 $\mathcal{H}(\boldsymbol{\pi},\boldsymbol{\kappa})$,其 C下的像 $t\to(\boldsymbol{\pi}'(t),\boldsymbol{\kappa}'(t))=C(\boldsymbol{\pi}(t),\boldsymbol{\kappa}(t))$是"同一个"哈密顿量(指 $\mathcal{H}(\boldsymbol{\pi}',\boldsymbol{\kappa}')\overset{\mathrm{def}}{=}\mathcal{H}(C^{-1}(\boldsymbol{\pi}',\boldsymbol{\kappa}'))$)的方程[12]的解,则坐标变换是正则的[②]。

利用函数 $\mathcal{H}$ 的任意性(指方程[12]不足以惟一地确定哈密顿量——译者注)容易得到正则坐标变换的条件,可简单地表示为其雅可比矩阵

$$\boldsymbol{L}=\begin{pmatrix}\boldsymbol{A} & \boldsymbol{B}\\ \boldsymbol{C} & \boldsymbol{D}\end{pmatrix}$$

① 此处原文有打印错误——译者注。

② 指方程[12]不能惟一地确定哈密顿量——译者注。

$$A_{ij}=\partial_{\pi_j}\pi'_i,\qquad B_{ij}=\partial_{k_j}\pi'_i,\qquad C_{ij}=\partial_{\pi_j}k'_i,\qquad D_{ij}=\partial_{k_j}k'_i \qquad [15]$$
$$i,j=1,\cdots,\ell$$

的一个必要和充分的性质。用

$$\boldsymbol{E}=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$$

表示由 4 个 $\ell\times\ell$ 方块等于零矩阵或如所示那样的正负单位矩阵所组成的 $2\ell\times2\ell$ 矩阵,上标 T 表示转置矩阵,则映射为正则的条件为

$$\boldsymbol{L}^{-1}=\boldsymbol{E}\boldsymbol{L}^{\mathrm{T}}\boldsymbol{E}^{\mathrm{T}}\text{或}\boldsymbol{L}^{-1}=\begin{pmatrix}\boldsymbol{D}^{\mathrm{T}} & -\boldsymbol{B}^{\mathrm{T}}\\ -\boldsymbol{C}^{\mathrm{T}} & \boldsymbol{A}^{\mathrm{T}}\end{pmatrix} \qquad [16]$$

这直接意味着 $\det\boldsymbol{L}=\pm1$。实际上,从方程[16]可知 $\det\boldsymbol{L}=1$。方程[16]等价于 4 个关系 $\boldsymbol{A}\boldsymbol{D}^{\mathrm{T}}-\boldsymbol{B}\boldsymbol{C}^{\mathrm{T}}=1$,$-\boldsymbol{A}\boldsymbol{B}^{\mathrm{T}}+\boldsymbol{B}\boldsymbol{A}^{\mathrm{T}}=0$,$\boldsymbol{C}\boldsymbol{D}^{\mathrm{T}}-\boldsymbol{D}\boldsymbol{C}^{\mathrm{T}}=1$ 和 $-\boldsymbol{C}\boldsymbol{B}^{\mathrm{T}}+\boldsymbol{D}\boldsymbol{A}^{\mathrm{T}}=1$。因为第一和第四个关系是相同的,故这些关系可表示为

$$\{\pi'_i,k'_j\}=\delta_{ij},\qquad \{\pi'_i,\pi'_j\}=0,\qquad \{k'_i,k'_j\}=0 \qquad [17]$$

这里对任意的函数 $F(\pi,\kappa)$和 $G(\pi,\kappa)$,**泊松括号**

$$\{F,G\}(\boldsymbol{\pi},\boldsymbol{\kappa})\overset{\text{def}}{=}\sum_{k=1}^{\ell}\partial_{\pi_k}F(\pi,\boldsymbol{\kappa})\partial_{K_k}G(\boldsymbol{\pi},\boldsymbol{\kappa})-\partial_{K_k}F(\boldsymbol{\pi},\boldsymbol{\kappa})\partial_{\pi_k}G(\boldsymbol{\pi},\boldsymbol{\kappa}) \qquad [18]$$

满足**雅可比恒等式**,即对于相空间任意 3 个函数 F,G,Q, 有 $\{\{F,G\},Q\}+\{\{G,Q,\},F\}+\{\{Q,F\},G\}=0$。下述结果是非常有用的:若 $t\to(\boldsymbol{p}(t),\boldsymbol{q}(t))=S_t(\boldsymbol{p},\boldsymbol{q})$是关于哈密顿量 $\mathcal{H}$ 的哈密顿方程的解,给定任意的观测量 $F(\boldsymbol{p},\boldsymbol{q})$,它的演化,$F(t)\overset{\text{def}}{=}F(\boldsymbol{p}(t),\boldsymbol{q}(t))$满足$\partial_t F(\boldsymbol{p}(t),\boldsymbol{q}(t))=\{\mathcal{H},F\}(\boldsymbol{p}(t),\boldsymbol{q}(t))$。要求这个等式对所有观测量成立即是要求$t\to(\boldsymbol{p}(t),\boldsymbol{q}(t))$是关于 $\mathcal{H}$ 的哈密顿方程的解。

令 $C:U\to U'$是一在两个 2ℓ 维的开集之间的光滑的且光滑地可逆的变换:$C(\boldsymbol{\pi},\boldsymbol{\kappa})=(\boldsymbol{\pi}',\boldsymbol{\kappa}')$。假如有一定义在合适区域 W 上的函数 $\Phi(\boldsymbol{\pi}',\boldsymbol{\kappa})$满足,

$$\mathcal{C}(\boldsymbol{\pi},\boldsymbol{\kappa})=(\boldsymbol{\pi}',\boldsymbol{\kappa}')\Rightarrow\begin{cases}\boldsymbol{\pi}=\partial_k\Phi(\boldsymbol{\pi}',\boldsymbol{\kappa})\\ \boldsymbol{\kappa}'=\partial_{\pi'}\Phi(\boldsymbol{\pi}',\boldsymbol{\kappa})\end{cases} \qquad [19]$$

则 $\mathcal{C}$是正则的。这是因为方程[19]意味着如果 $\boldsymbol{\kappa},\boldsymbol{\pi}'$被改变,且 $\boldsymbol{\pi},\boldsymbol{\kappa}',\boldsymbol{\pi}',\boldsymbol{\kappa}$ 通过 $\mathcal{C}(\boldsymbol{\pi},\boldsymbol{\kappa})=(\boldsymbol{\pi}',\boldsymbol{\kappa}')$相联系,则 $\boldsymbol{\pi}\cdot\mathrm{d}\boldsymbol{\kappa}+\boldsymbol{\kappa}'\cdot\mathrm{d}\boldsymbol{\pi}'=\mathrm{d}\Phi(\boldsymbol{\pi}',\boldsymbol{\kappa})$,即有

$$\boldsymbol{\pi}\cdot\mathrm{d}\boldsymbol{\kappa}-\mathcal{H}(\boldsymbol{\pi},\boldsymbol{\kappa})\mathrm{d}t\equiv\boldsymbol{\pi}'\cdot\mathrm{d}\boldsymbol{\kappa}'-\mathcal{H}(\mathcal{C}^{-1}(\boldsymbol{\pi}',\boldsymbol{\kappa}'))\mathrm{d}t+\mathrm{d}\Phi(\boldsymbol{\pi}',\boldsymbol{\kappa})-\mathrm{d}(\boldsymbol{\pi}'\cdot\boldsymbol{\kappa}') \qquad [20]$$

意思是哈密顿量 $\mathcal{H}'(\boldsymbol{p},\boldsymbol{q})$和 $\mathcal{H}'(\boldsymbol{p}',\boldsymbol{q}')\overset{\text{def}}{=}\mathcal{H}(\mathcal{C}^{-1}(\boldsymbol{p}',\boldsymbol{q}'))$的哈密顿作用量 $\mathcal{A}_{\mathcal{H}}$ 和 $\mathcal{A}_{\mathcal{H}'}$,如果针对运动$(\boldsymbol{p}(t),\boldsymbol{q}(t))$和$(\boldsymbol{p}'(t),\boldsymbol{q}'(t))=\mathcal{C}(\boldsymbol{p}(t),\boldsymbol{q}(t))$计算,则相差一个常数。

这个常数只分别取决于相应的初始值和终值$(\boldsymbol{p}(t_1),\boldsymbol{q}(t_1))$和$(\boldsymbol{p}(t_2),\boldsymbol{q}(t_2))$,以及$(\boldsymbol{p}'(t_1),\boldsymbol{q}'(t_1))$和$(\boldsymbol{p}'(t_2),\boldsymbol{q}'(t_2))$;因此,如果$(\boldsymbol{p}(t),\boldsymbol{q}(t))$使得 $\mathcal{A}_{\mathcal{H}}$ 取极值,则$(\boldsymbol{p}'(t),\boldsymbol{q}'(t))=\mathcal{C}(\boldsymbol{p}(t),\boldsymbol{q}(t))$ 也使得 $\mathcal{A}_{\mathcal{H}'}$取极值。这样,若 $t\to(\boldsymbol{p}(t),\boldsymbol{q}(t))$是哈密顿量 $\mathcal{H}(\boldsymbol{p},\boldsymbol{q})$对应的哈密顿方程的解,则 $t\to(\boldsymbol{p}'(t),\boldsymbol{q}'(t))=\mathcal{C}(\boldsymbol{p}(t),\boldsymbol{q}(t))$一定是哈密顿量 $\mathcal{H}'(\boldsymbol{p}',\boldsymbol{q}')=\mathcal{H}(\mathcal{C}^{-1}(\boldsymbol{p}',\boldsymbol{q}'))$对应的哈密顿方程的解。因此,该变换是正则的。函数 Φ 被称为它的生成函数。

方程[19]提供了一个构造正则映射的途径。假设函数 $\Phi(\boldsymbol{\pi}',\boldsymbol{\kappa})$定义在某个区域 W 上,令

$$\begin{cases}\boldsymbol{\pi}=\partial_k\Phi(\boldsymbol{\pi}',\boldsymbol{\kappa})\\ \boldsymbol{\kappa}'=\partial_{\pi'}\Phi(\boldsymbol{\pi}',\boldsymbol{\kappa})\end{cases}$$

对第一个方程求逆得到 $\boldsymbol{\pi}'=\boldsymbol{\Xi}(\boldsymbol{\pi},\boldsymbol{\kappa})$,把得到的 $\boldsymbol{\pi}'$ 代入第二个方程,则映射 $\mathcal{C}(\boldsymbol{\pi},\boldsymbol{\kappa})=(\boldsymbol{\pi}',\boldsymbol{\kappa}')$ 就被定义在某个域(前述的运算在其上可以操作)上了;如果这个域是开的且不为空,则 $\mathcal{C}$ 是正则映射。

基于类似的理由,如果 $\Gamma(\kappa,\kappa')$ 是定义在某个域上的函数,令 $\pi=-\partial_{\kappa}\Gamma(\boldsymbol{\kappa},\boldsymbol{\kappa}')$,$\boldsymbol{\pi}'=\partial_{\kappa'}\Gamma(\kappa,\kappa')$,解第一个关系式,表为 $\boldsymbol{\kappa}'=\Delta(\boldsymbol{\pi},\boldsymbol{\kappa})$,代入第二个关系式,则映射 $(\boldsymbol{\pi}',\boldsymbol{\kappa}')=\mathcal{C}(\boldsymbol{\pi},\boldsymbol{k})$ 就被定义在某个域上(所言的操作可以进行);如果该域是开的,非空的,则 $\mathcal{C}$ 是正则映射。

同样,正则变换可以由预先给定的函数 $F(\boldsymbol{\pi},\boldsymbol{\kappa}')$ 或 $G(\boldsymbol{\pi},\boldsymbol{\pi}')$ 构造。最一般情况下的正则映射都可由上述 4 种方式局域地生成(即靠近相空间给定点),当然也可能包含一些如把一对坐标 (π_i,k_i) 变换成 $(-k_i,\pi_i)$ 那样的"平凡"正则映射。出现平凡映射的必然性可以追溯到齐次正则映射 $\boldsymbol{\pi}\cdot\mathrm{d}\boldsymbol{\kappa}=\boldsymbol{\pi}'\cdot\mathrm{d}\boldsymbol{\kappa}'$(即全等映射,参见下文或[49]中非平凡的例子)的存在,它使得作用量守恒因而是正则的,但它明显地不能由函数 $\Phi(\boldsymbol{\kappa},\boldsymbol{\kappa}')$ 生成,虽然它可以由依赖于 $\boldsymbol{\pi}',\boldsymbol{\kappa}$ 的函数生成。

齐次正则映射的简单例子是坐标 $\boldsymbol{q}$ 变化到 $\boldsymbol{q}'=\boldsymbol{R}(\boldsymbol{q})$ 的映射,相应的动量 $\boldsymbol{p}$ 线性地变化到 $\boldsymbol{p}'=(\partial_{\boldsymbol{q}}\boldsymbol{R}(\boldsymbol{q}))^{-1\mathrm{T}}\boldsymbol{p}$;实际上这个映射是由函数 $F(\boldsymbol{p}',\boldsymbol{q})\overset{\text{def}}{=}\boldsymbol{p}'\cdot\boldsymbol{R}(\boldsymbol{q})$ 生成的。

举例来说,考虑"笛卡儿-极坐标"映射 $(q_1,q_2)\leftrightarrow(\rho,\theta)$,$(\rho,\theta)$ 是 $\boldsymbol{q}$ 的极坐标(即 $\rho=\sqrt{q_1^2+q_2^2}$,$\theta=\arctan(q_2/q_1)$),记 $\boldsymbol{n}\overset{\text{def}}{=}\boldsymbol{q}/|\boldsymbol{q}|=(n_1,n_2)$,$\boldsymbol{t}=(-n_2,n_1)$。令 $p_\rho\overset{\text{def}}{=}\boldsymbol{p}\cdot\boldsymbol{n}$,$p_\theta\overset{\text{def}}{=}\rho\boldsymbol{p}\cdot\boldsymbol{t}$,映射 $(p_1,p_2,q_1,q_2)\leftrightarrow(p_\rho,p_\theta,\rho,\theta)$ 是齐次正则的(因为 $\boldsymbol{p}\cdot d\boldsymbol{q}=\boldsymbol{p}\cdot\boldsymbol{n}\mathrm{d}\rho+\boldsymbol{p}\cdot\boldsymbol{t}\rho\mathrm{d}\theta=p_\rho\cdot\mathrm{d}\rho+p_\theta\cdot\mathrm{d}\theta$)。

另一个正则变换的例子是定义在平面 R^2 内的一个开集上的面积守恒的映射 $(p,q)\leftrightarrow(p',q')$,因为这种情况下矩阵 $\boldsymbol{A},\boldsymbol{B},\boldsymbol{C},\boldsymbol{D}$ 都是数字,且满足 $\boldsymbol{AD}-\boldsymbol{BC}=1$,因此式[16]成立。

欲知更多的细节,读者可参阅 Landau,Lifshitz(1976) 和 Gallavotti(1983)。

二次型

最简单的力学系统是二次型可积的。比如定义在 R^2 上的哈密顿量

$$\mathcal{H}(p,q)=\frac{1}{2m}p^2+V(q) \qquad [21]$$

产生初始值为 $q_0,\dot{q}_0$,且 $\mathcal{H}(p_0,q_0)=E$,即 $\frac{1}{2m}p_0{}^2+V(q_0)=E$ 的运动 $t\to q(t)$,它满足 $\dot{q}(t)=\pm\sqrt{\frac{2}{m}(E-V(q(t))}$。如果方程 $E=V(q)$ 只有两个解 $q_-(E)<q_+(E)$,且 $|\partial_q V(q_-(E))|>0$,则运动是周期的,周期为

$$T(E)=2\int_{q_-(E)}^{q_+(E)}\frac{\mathrm{d}x}{\sqrt{(2/m)(E-V(x))}} \qquad [22]$$

初始值为 $q_0=q_-(E)$,$\dot{q}_0=0$ 的特解可表示为 $Q(t)$,它是解析函数(由关于常微分方程的一般正则性定理可知),对 $0\leqslant t\leqslant T/2$ 或 $T/2\leqslant t\leqslant T$ 它可分别由

$$t=\int_{q_-(E)}^{Q(t)}\frac{\mathrm{d}x}{\sqrt{(2/m)(E-V(x))}} \qquad [23a]$$

或

$$\iota = \frac{T}{2} - \int_{q_1(E)}^{Q(t)} \frac{\mathrm{d}x}{\sqrt{(2/m)(E-V(x))}} \qquad [23b]$$

给出。能量为 E 的一般解有形式 $q(t)=Q(t_0+t)$,其中 t_0 由 $q_0(t)=Q(t_0)$,$\dot{q}_0(t)=\dot{q}(t_0)$定义,即标准解 $Q(t)$到达新的运动初始值所需的时间。

如果 V 的导数在极点之一上为零,或者至少两个解 $q_\pm(E)$中的一个不存在,则运动是非周期的,甚至可能是无界的,但它依然可以用[22]那样的积分表示。如果势能 V 关于 q 是周期的,且变量 q 在一个圆上变化,则本质上所有的解都是周期的,例外只有当能量为 E 且 $V(q)=E$ 时,有 V 的导数为零的解。

典型的例子有谐振子、单摆和开普勒振子。设 m,ω,g,h,G,k 都是正的常量,相应的哈密顿量分别为

$$\left.\begin{aligned} &\frac{p^2}{2m}+\frac{1}{2}m\omega^2q^2 \\ &\frac{p^2}{2m}+mg\left(1-\cos\frac{q}{h}\right) \\ &\frac{p^2}{2m}-mk\,\frac{1}{|q|}+m\,\frac{G^2}{2q^2} \end{aligned}\right\} \qquad [24]$$

开普勒振子哈密顿量中的势能有奇点 $q=0$,但如果 $G\neq0$,能量守恒禁止轨道过分靠近 $q=0$,因此这个奇点是不相关的。

式[23]中的积分称为**二次型**,式[21]中的系统因此**是二次型可积系统**。对于这样的系统,至少当运动是周期性的时候,最好用新的坐标描述从而使周期性看起来更明显。若$V(q)=E$ 只有两个解 $q_\pm(E)$且$\mp V'(q_\pm(E))>0$,**能量-时间坐标** E,τ 可用来替代 $q,\dot{q}$ 或 p,q,这里 τ 是标准解 $\iota\to Q(t)$到达指定值所需的时间,有 $Q(\tau)=q,\dot{q}(\tau)=\dot{q}$。在这样的坐标系里,运动简单地就是$(E,\tau)\to(E,\tau+t)$,当然,变量 τ 是在半径为 $T/2\pi$ 的圆上变化。变量 E,τ 是一类极坐标,这一点可以通过对[24]中的系统在 p,q 平面上画出等能量线看出来,见图 1。

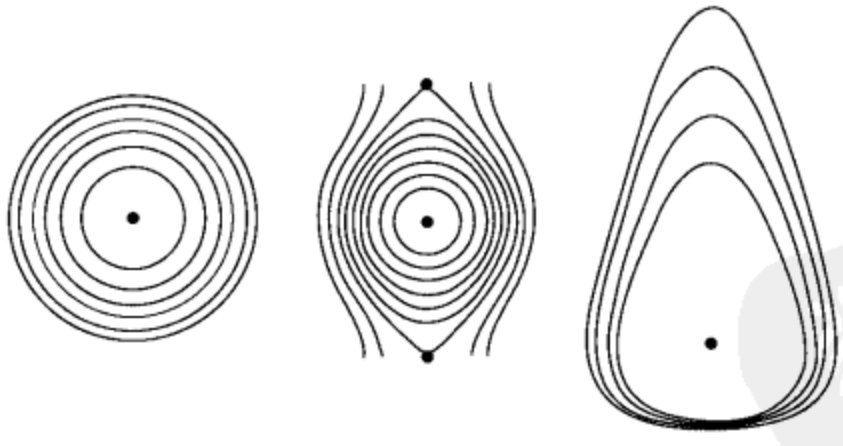

图 1　谐振子、单摆和开普勒运动的能级。

对于谐振子,所有的轨道都是周期的;对于单摆,除了把振动运动(第二个图中的闭合曲线)同转动运动(明显开放的曲线)分割开来的那一个运动(它实际上是在闭合曲线上,如果坐标 q,即图 1 中的垂直坐标,被认为有周期 $2\pi h$)外,都是周期性的。而在开普勒振子的情况下,只有能量为负的轨道才是周期的,一些这样的轨道在图 1 中画出来了。图中的单个黑点为相空间中的平衡点。

相空间中周期性运动的区域是具有拓扑结构$\bigcup_{u\in U}(\{u\}\times C_u)$的点$(p,q)$的集合,其中$u$是在开集$U$(比如能量值的集合)中变化的坐标,而$C_u$是其点$(p,q)$可以用坐标表示的闭合曲线(比如,从任意具有同样能量的固定点到(p,q)所需的时间)。

在式[24]的情形下,如果"径向"坐标选为能量,则关于谐振子的点集U为$(0,\infty)$,关于单摆的点集U为$(0,2mg)$或$(2mg,\infty)$,关于开普勒振子的点集U为$\left(-\frac{1}{2}mk^2/G^2,0\right)$。作为参照运动的固定点,在所有情形下,都可以选为形式$(0,q_0)$,时间坐标t_0由式[23]给出。

注意到能量-时间坐标是正则的。例如,在点(p_0,q_0)附近,且如果$p_0>0$,则令

$$S(q,E)=\int_{q_0}^{q}\sqrt{2m(E-V(x))}\,\mathrm{d}x \qquad [25]$$

然后可以验证,如果(p,q)是(E,t)同一点的坐标,则$p=\partial_q S(q,E)$和$t=\partial_E S(q,E)$是恒等式,由此式[20]表达的判据得到满足。

可以方便地通过用变量$\alpha=(2\pi/T(E))t$替代时间,用能量的任何可逆函数替代能量,对坐标加以标准化。

自然地,可以找寻这样的坐标,$A=A(E)$,使得映射$(p,q)\to(A,\alpha)$为一正则映射。这一点很容易做到。函数

$$\hat{S}(q,A)=\int_{q_0}^{q}\sqrt{2m(E(A)-V(x))}\,\mathrm{d}x \qquad [26]$$

(局域地)产生了$p=\sqrt{2m(E(A)-V(q))}$和$\alpha=E'(A)\int_0^q\frac{\mathrm{d}x}{\sqrt{2m^{-1}(E(A)-V(x))}}$之间的对应,因此,由判据式[20],如果$E'(A)=\frac{2\pi}{T(E(A))}$,即如果$A'(E)=T(E)/2\pi$,则坐标$(A,\alpha)$是正则的。由式[22],$A(E)$可表示为

$$A=\frac{1}{2\pi}2\int_{q_-(E)}^{q_+(E)}\sqrt{2m(E-V(q))}\,\mathrm{d}q\equiv\frac{1}{2\pi}\oint p\mathrm{d}q \qquad [27]$$

这里最后的积分扩展到能量E的闭合曲线上,见图1。**作用量-角坐标**(A,α)定义在周期运动所覆盖的相空间的开区域上,对于作用量-角坐标,此区域有形式$W=J\times\mathbb{T}$,是一个开区间J和一个一维"圆环面"$\mathbb{T}=[0,2\pi]$(即单位圆)的乘积。

欲知更多的细节,读者可参阅 Landau, Lifshitz(1976), Arnol'd(1989) 和 Gallavotti(1983)。

准周期性与可积性

一个哈密顿量被称为在相空间的开区域$W\subset T^*(M)$内可积的,如果

(1) 有一个解析的且非奇异的(即雅可比行列式不为零)的坐标变换$(\boldsymbol{p},\boldsymbol{q})\to(\boldsymbol{I},\boldsymbol{\varphi})$把$W$映射到形式为$\mathcal{I}\times\mathbb{T}^l$的集合上,其中$\mathcal{I}\subset\mathbb{R}^l$(开的);

(2) 相空间上的流$t\to S_t(\boldsymbol{p},\boldsymbol{q})$变换成$(\boldsymbol{I},\boldsymbol{\varphi})\to(\boldsymbol{I},\boldsymbol{\varphi}+\boldsymbol{\omega}(\boldsymbol{I})t)$,$\boldsymbol{\omega}(\boldsymbol{I})$是$\mathcal{I}$上的光滑函数。

这意味着,在合适的坐标系(称为"积分坐标系")中,系统看起来由一组l个其坐标$\boldsymbol{\varphi}=(\varphi_1,\cdots,\varphi_l)$沿单位圆运动的点组成,其角速度$\boldsymbol{\omega}(\boldsymbol{I})=(\boldsymbol{\omega}_1(\boldsymbol{I}),\cdots,\boldsymbol{\omega}_l(\boldsymbol{I}))$由初始条件

对应的作用量决定。

一个区域 W(在积分坐标 $\boldsymbol{I},\boldsymbol{\varphi}$ 中形式为 $I\times\mathbb{T}^l$)上的可积系统,如果行列式 $\partial_I\boldsymbol{\omega}(\boldsymbol{I})\neq 0$,称为**非等时的**。如果 $\boldsymbol{\omega}(\boldsymbol{I})\equiv\boldsymbol{\omega}$,不依赖于 $\boldsymbol{I}$,则称为等时性的。一个系统如果在坐标 $(\boldsymbol{I},\boldsymbol{\varphi})$ 中有频率谱 $\boldsymbol{\omega}(\boldsymbol{I})$,或有**频率** $\omega(I)/2\pi$ 表示,则该运动称为**准周期的**。

显然,一个可积系统有 l 个独立的运动常数 $\boldsymbol{I}=(I_1,\cdots,I_l)$;对每一个 $\boldsymbol{I}$ 的选择,其他的坐标在"标准的" l 维圆环面 $\mathbb{T}^l$ 上变化,因此可以说,一个有可积性的相空间区域被**分叶**成以运动常数 $\boldsymbol{I}\in\mathcal{I}$ 的不同值为参数的 l 维不变圆环面 $T(I)$ 的叶状结构。

如果一个可积系统是非等时的,则它是**正则可积**的,即可以在 W 上定义正则的坐标变换 $(\boldsymbol{p},\boldsymbol{q})\to\mathcal{C}(\boldsymbol{A},\boldsymbol{\alpha})$ 把 W 映射到 $J\times\mathbb{T}^l$ 上,从而对合适的 h 有 $\mathcal{H}(\mathcal{C}(\boldsymbol{A},\boldsymbol{\alpha}))=h(\boldsymbol{A})$。如果 $\boldsymbol{\omega}(\boldsymbol{A})\overset{\text{def}}{=}\partial_A h(\boldsymbol{A})$,运动方程变为

$$\dot{\boldsymbol{A}}=0,\qquad \dot{\alpha}=\boldsymbol{\omega}(\boldsymbol{A}) \tag{28}$$

给定一个可积的非等时系统一个坐标系 $(\boldsymbol{I},\boldsymbol{\varphi})$,则其作用量-角坐标可以原则上通过一个经典的程序来构造(需要一些额外的假设)。令 $\gamma_1,\cdots,\gamma_l$ 为 $\mathbb{T}^l$ 上的 l 个相互拓扑独立的圆,令 $\gamma_i(\boldsymbol{I})=\{\boldsymbol{\varphi}\,|\,\varphi_1=\varphi_2=\cdots=\varphi_{i-1}=\varphi_{i+1}=\cdots=0,\varphi_i\in[0,2\pi]\}$,取

$$A_i(\boldsymbol{I})=\frac{1}{2\pi}\oint_{\gamma_i(\boldsymbol{I})}\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{q} \tag{29}$$

如果映射 $\boldsymbol{I}\leftrightarrow\boldsymbol{A}(\boldsymbol{I})$ 是解析可逆的,如 $\boldsymbol{I}=\boldsymbol{I}(\boldsymbol{A})$,则函数

$$S(\boldsymbol{A},\boldsymbol{\varphi})=(\lambda)\int_0^{\varphi}\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{q} \tag{30}$$

是定义良好的,其中积分是沿任何连接点 $(p(\boldsymbol{I}(\boldsymbol{A}),0),q(\boldsymbol{I}(\boldsymbol{A}),0))$ 和点 $(p(\boldsymbol{I}(\boldsymbol{A}),\boldsymbol{\varphi}),q(I(\boldsymbol{A}),\boldsymbol{\varphi}))$ 且是在由 $\boldsymbol{I}(\boldsymbol{A})$ 参数化的圆环面上的路径 λ 上进行的。

证明式[30]确实定义了一个只是关于变量 $\boldsymbol{A},\boldsymbol{\varphi}$ 的函数之关键点是,非等时性意味着泊松括号为零(比较式[18]),$\{I_i,I_j\}=0$(因此有 $\{A_i,A_j\}=\sum_{h,k}\partial_{I_k}A_i\partial_{I_h}A_j\{I_k,I_h\}=0$)。可以验证,性质 $\{I_i,I_j\}=0$ 就是由变化 q 但约束 p 从而使得 $(\boldsymbol{p},\boldsymbol{q})$ 保持在 $\boldsymbol{I}=$常数的曲面上(即在固定 $\boldsymbol{I}$ 值的点之不变圆环面上)所得到的积分形式 $\boldsymbol{p}\cdot\mathrm{d}\boldsymbol{q}$ 的可积条件。

后一性质是充分必要的,它使得函数 $S(\boldsymbol{A},\boldsymbol{\varphi})$ 是定义良好的(即不依赖于积分路径 λ),相差一个常量其形式为 $\sum_i 2\pi n_i A_i$,其中 $\boldsymbol{n}=(n_1,\cdots,n_l)$ 是整数。

作用量-角变量可由 $S(\boldsymbol{A},\boldsymbol{\varphi})$ 作为生成函数的坐标正则变换得到,即令

$$\alpha_i=\partial_{A_i}S(\boldsymbol{A},\boldsymbol{\varphi}),\qquad I_i=\partial_{\varphi_i}S(\boldsymbol{A},\boldsymbol{\varphi}) \tag{31}$$

因为 $S(\boldsymbol{A},\boldsymbol{\varphi})$ 的计算约化为积分,可以看作是针对一维情形已经讨论过的二次型的自然推广,这样的系统称为**二次型可积的**。前述的构造是更一般的 **Arnol′d-Liouville 定理**的一个版本。

实际上式[29]与式[30]的计算可能是非常困难的,在许多情况下(甚至像单摆一样基本)问题分析导致了在不同领域中的重大进展,比如在特殊函数和群论方面。

一般地,相空间中的任何表面,若微分形式 $p\cdot\mathrm{d}q$ 是局域可积的,就称为**拉格朗日流形**;因此,一个非等时可积系统的不变圆环面是拉格朗日流形。

如果一个可积系统是非等时的,它最多只能有 l 个独立的运动常数。进一步地,它就不能允许维度大于 l 的不变圆环面。因此 l 维不变圆环面是最大的。

当然,维度小于 ℓ 的不变圆环面可以存在。这出现在变量 $\boldsymbol{I}$ 使得频率 $\boldsymbol{\omega}(\boldsymbol{I})$ 之间有非平凡的有理关系,即存在一个分量为整数的矢量 $\boldsymbol{v}\in\mathcal{Z}$, $\boldsymbol{v}=(v_1,\cdots,v_\ell)\neq 0$,使得

$$\boldsymbol{\omega}(\boldsymbol{I})\cdot\boldsymbol{v}=\sum_i \omega_i(\boldsymbol{I})v_i=0 \qquad [32]$$

在这种情况下,不变圆环面 $\mathcal{T}(\boldsymbol{I})$ 是**共振的**。如果系统是非等时的,则 $\det\partial_I\boldsymbol{\omega}(\boldsymbol{I})\neq 0$,因此共振圆环面和运动常数 $\boldsymbol{I}$ 的一些值相联系。这些值在空间 $\mathcal{I}$ 中形成一个测度为零的、非空的、稠的集合。

等时性的系统的例子是谐振子构成的系统,即哈密顿量为

$$\sum_{i=1}^{\ell}\frac{1}{2m}p_i^2+\frac{1}{2}\sum_{i,j}^{1,\ell}c_{ij}q_iq_j$$

的系统,这里矩阵 c_{ij} 是正定的矩阵①。这个等时系统的频率 $\boldsymbol{\omega}=(\omega_1,\cdots,\omega_\ell)$ 为矩阵 $m_i{}^{-1/2}c_{ij}m_j{}^{1/2}$ 的特征值的平方。它在点 $\boldsymbol{x}=(\boldsymbol{p},\boldsymbol{q})\in\mathbb{R}^{2\ell}$ 的区域 W 上是可积的,从而,关于上述矩阵的所有本征矢量 v_β, $\beta=1,\cdots,\ell$,若设定

$$\boldsymbol{A}_\beta=\frac{1}{2\omega_\beta}\left(\left(\sum_{i=1}^{\ell}\boldsymbol{v}_{\beta,i}\frac{p_i}{\sqrt{m_i}}\right)^2+\omega_\beta^2\left(\sum_{i=1}^{\ell}\boldsymbol{v}_{\beta,i}\frac{p_i}{\sqrt{m_i^{-1}}}\right)^2\right)$$

则矢量 $\boldsymbol{A}$ 的所有分量>0。

尽管这个系统是等时性的,它依然可采用一个正则的作用量-角的坐标系,在其中它的哈密顿量取简单的形式

$$h(\boldsymbol{A})=\sum_{\beta=1}^{\ell}\bar{\omega}_\beta\boldsymbol{A}_\beta\equiv\boldsymbol{\omega}\cdot\boldsymbol{A} \qquad [33]$$

这里 $\alpha_\beta=-\arctan\left(\dfrac{\sum_{i=1}^{\ell}\dfrac{\boldsymbol{v}_{\beta,i}p_i}{\sqrt{m_i}}}{\sum_{i=1}^{\ell}\sqrt{m_i}\omega_\beta\boldsymbol{v}_{\beta,i}q_i}\right)$ 是共轭的角变量。

非等时系统的一个例子是**自由转子**或**自由轮子**,即 ℓ 个在半径为 R 的圆上不相互作用的质点或 ℓ 个不相互作用的半径为 R 的均匀"一致"同轴的轮子。如果 $J_i=m_iR^2$ 和 $J_i=(1/2)m_iR^2$ 分别是对应的转动惯量,且位置由 ℓ 个角度 $\boldsymbol{\alpha}=(\alpha_1,\cdots,\alpha_\ell)$ 给定,则角速度是角动量 $\boldsymbol{A}=(A_1,\cdots,A_\ell)$ 通过 $\omega_i=A_i/J_i$ 相联系的常量。哈密顿量和频谱分别为

$$h(\boldsymbol{A})=\sum_{i=1}^{\ell}\frac{1}{2J_i}A_i^2,\qquad \boldsymbol{\omega}(\boldsymbol{A})=\left(\frac{1}{J_i}A_i\right)_{i=1,\cdots,\ell} \qquad [34]$$

欲知更多的细节,读者可参阅 Landau, Lifshitz(1976), Gallavotti(1983), Arnol′d(1989)和 Fassò(1998)。

多维二次型:有心运动

几个重要的多维力学系统在相空间广大的区域内是正则二次型可积的。证实这一点只需表明,区域有一个分叶为维度等于自由度数(ℓ)的,由 ℓ 个内旋的运动常数 $\boldsymbol{I}$(即使得 $\{I_i,I_j\}=0$)加以参数化的的不变圆环面 $\mathcal{T}(\boldsymbol{I})$ 的叶状结构。这样,有可能的话,就可以用前节讨论的二次型来构造作用量-角变量。

上述的程序可以由关于单位质量的质点在有心力吸引下的平面运动的理论加以演

① 此处原文误为"矩阵 v"——译者注。

示。在极坐标系(ρ,θ)中,系统的拉格朗日量为

$$\mathcal{L}=\frac{m}{2}(\dot{\rho}^2+\rho^2\dot{\theta}^2)-V(\rho)$$

对运动的平面性要求不是强的限制,因为有心运动总是在一个平面内进行的。

由此,运动的方程为

$$\frac{\mathrm{d}}{\mathrm{d}t}m\rho^2\dot{\theta}=0$$

即$m\rho^2\dot{\theta}=G$是一个运动常量(就是角动量),且有

$$\dot{\rho}=-\partial_\rho V(\rho)+\partial_\rho\frac{m}{2}\rho^2\dot{\theta}^2=-\partial_\rho V(\rho)+\frac{G^2}{m\rho^3}\overset{\text{def}}{=}-\partial_\rho V_G(\rho)$$

然后由能量守恒得到第二个运动常量E

$$\frac{m}{2}\dot{\rho}^2+\frac{1}{2}\frac{G^2}{m\rho^2}+V(\rho)=E=\frac{1}{2m}p_\rho^2+\frac{1}{2m}\frac{p_\theta^2}{\rho^2}+V(\rho)\qquad[35]$$

方程的右边为系统的哈密顿量,可由$\mathcal{L}$得到,p_ρ和p_θ分别是ρ,θ的共轭动量,$p_\rho=m\dot{\rho}$,$p_\theta=m\rho^2\dot{\theta}$(注意$p_\theta=G$)。

假设$\rho^2V(\rho)\underset{\rho\to0}{\to}0$,如果$G>0$,则始于$\rho>0$的任何运动永远不会到达处于原点的奇点。再假设函数

$$V_G(\rho)\overset{\text{def}}{=}\frac{1}{2}\frac{G^2}{m\rho^2}+V(\rho)$$

只有极小值$E_0(G)$,没有极大值也没有水平的弯折,且当$\rho\to\infty$时它趋于极限$E_\infty(G)\leqslant\infty$,那么系统在区域$W=\{(\boldsymbol{p},\boldsymbol{q})\mid E_0(G)<E<E_\infty(G),G\neq0\}$上是可积的。

这一点可以通过引入方程$m\ddot{\rho}=-\partial_\rho V_G(\rho)$在能量为$E_0(G)<E<E_\infty(G)$和$t=0$时的初始条件为$\rho=\rho_{E,-}(G)$,$\dot{\rho}=0$情况下之"标准"周期解$t\to R(t)$加以验证。这里$\rho_{E,\pm}(G)$是方程$V_G(\rho)=E$的两个解,参见"二次型"一节。$t$的周期性解析函数的周期是

$$T(E,G)=2\int_{\rho_{E,-}(G)}^{\rho_{E,+}(G)}\frac{\mathrm{d}x}{\sqrt{(2/m)(E-V_G(x))}}$$

在区间$0\leqslant t\leqslant\frac{1}{2}T(E,G)$或$\frac{1}{2}T(E,G)\leqslant t\leqslant T(E,G)$内的函数$R(t)$分别由二次型

$$t=\int_{\rho_{E,-}(G)}^{R(t)}\frac{\mathrm{d}x}{\sqrt{(2/m)(E-V_G(x))}}\qquad[36a]$$

或

$$t=\frac{T(E,G)}{2}-\int_{\rho_{E,+}(G)}^{R(t)}\frac{\mathrm{d}x}{\sqrt{(2/m)(E-V_G(x))}}\qquad[36b]$$

给出。$R(t)$的解析正则性由关于$\ddot{\rho}$的微分方程的一般存在性、惟一性和正则性定理保证。

给定具有能量E和角动量G的初始值$\rho_0,\dot{\rho}_0,\theta_0,\dot{\theta}_0$,定义$t_0$时刻$R(t_0)=\rho_0$,$\dot{R}(t_0)=\dot{\rho}_0$,则$\rho(t)=R(t+t_0)$,$\theta(t)$可由第二个二次型

$$\theta(t)=\theta_0+\int_0^t\frac{G}{mR(t'+t_0)^2}\mathrm{d}t'$$

计算。因此,可以使用运动坐标E,G,t_0(它们决定了$\rho_0,\dot{\rho}_0,\dot{\theta}_0$)和某个第四坐标,这第四

个坐标决定 θ_0,它可以是 θ_0 本身,但也可以方便地通过第二个二次型如下确定。

函数 $Gm^{-1}R(t)^{-2}$ 是周期为 $T(E,G)$ 的函数,它可以表示为傅里叶级数

$$\chi_0(E,G)+\sum_{k\neq 0}\chi_k(E,G)\exp\left(\frac{2\pi}{T(E,G)}\mathrm{i}tk\right)$$

关于 $\theta(t)$ 的二次型可以由级数积分求出。令

$$\bar{\theta}(t_0)\overset{\text{def}}{=}\frac{T(E,G)}{2\pi}\sum_{k\neq 0}\frac{\chi_k(E,G)}{k}\exp\left(\frac{2\pi}{T(E,G)}\mathrm{i}t_0k\right)$$

且令 $\varphi_1(0)=\theta_0-\bar{\theta}(t_0)$,表达式

$$\theta(t)=\theta_0+\int_0^t\frac{G}{mR(t'+t_0)^2}\mathrm{d}t'$$

变成

$$\varphi_1(t)=\varphi_1(0)+\chi_0(E,G)t \qquad [37]$$

因此系统是可积的,其谱函数为 $\boldsymbol{\omega}(E,G)=(\omega_0(E,G),\omega_1(E,G))\equiv(\omega_0,\omega_1)$,其中 $\omega_0\overset{\text{def}}{=}\frac{2\pi}{T(E,G)}$,$\omega_1\overset{\text{def}}{=}\chi_0(E,G)$。因为 $\boldsymbol{I}=(E,G)$ 是运动常数,且角度 $\boldsymbol{\varphi}=(\varphi_0,\varphi_1)$ 可以写为

$$\varphi_0\overset{\text{def}}{=}\omega_0t_0,\quad \varphi_1\overset{\text{def}}{=}\theta_0-\bar{\theta}(t_0)$$

所以对于固定的 E,G,运动在二维圆环面 $\mathcal{T}(E,G)$(φ_0,φ_1 是其角参数)上进行。

在非等时的情况下,即当 $\det\partial_{E,G}\boldsymbol{\omega}(E,G)\neq 0$,同 $(p_\rho,\rho,p_\theta,\theta)$ 共轭的正则作用量-角变量可以用圆环面 $\mathcal{T}(E,G)$ 上的两个圆 γ_1,γ_2 通过式[29],式[30]来构造。如下的选取是方便的。

(1)γ_1 为由点 $\rho=x,\theta=0$ 组成的圆。圆的上半部($p_\rho\geqslant 0$)由 $\rho_{E,-}(G)\leqslant x\leqslant\rho_{E,+}(G)$,$p_\rho=\sqrt{2m(E-V_G(x))}$ 和 $\mathrm{d}\theta=0$ 组成;

(2)γ_2 为由点 $\rho=\mathrm{const},\theta\in[0,2\pi]$ 组成的圆,在其上 $\mathrm{d}\rho=0$,$p_\theta=G$,由此可得到

$$\left.\begin{aligned}A_1&=\frac{2}{2\pi}\int_{\rho_{E,-}(G)}^{\rho_{E,+}(G)}\sqrt{2m(E-V_G(x))}\,\mathrm{d}x\\A_2&=G\end{aligned}\right\} \qquad [38]$$

根据一般性理论(比较前一节),从 $(p_\rho,\rho,p_\theta,\theta)$ 到作用量-角变量的正则坐标变换的生成函数(为了掌握其中的思想,假设 $p_\rho>0$)是

$$S(A_1,A_2,\rho,\theta)=G\theta+\int_{\rho_{E,-}}^{\rho}\sqrt{2m(E-V_G(x))}\,\mathrm{d}x \qquad [39]$$

用 ω_0,χ_0 表示的雅可比行列式 $\partial(E,G)/\partial(A,A_2)$ 由式[38],式[39]可以算出,为 $\begin{pmatrix}\omega_0 & \chi_0\\0 & 1\end{pmatrix}$。由此可知,$\partial_E S=t$,$\partial_G S=\theta-\bar{\theta}(t)-\chi_0't$。因此,根据式[31],

$$\alpha_1\overset{\text{def}}{=}\partial_{A_1}S=\omega_0t,\quad \alpha_2\overset{\text{def}}{=}\partial_{A_2}S=\theta-\bar{\theta}(t) \qquad [40]$$

且 (A_1,α_1),(A_2,α_2) 是作用量-角变量对。

欲知更多的细节,读者可参阅 Landau,Lifshitz(1976) 和 Gallavotti(1983)。

牛顿势与开普勒定律

非常重要的谐振子势和牛顿势并不满足非等时性,即 $\det\partial(\omega_0,\chi_0)/\partial(A_1,A_2)\neq 0$,或等价地,$\det\partial(\omega_0,\chi_0)/\partial(E,G)\neq 0$。但非等时性只是正则可积性的充分条件,因此有可能(确实如此)对上述两种情况由式[39]产生的正则变换能够对系统积分。之所以有这样的预期是因为这两个势能是非等时势的极限情况(例如,取 $\varepsilon\to 0$ 时的 $|q|^{2+\varepsilon}$ 和 $|q|^{-1-\varepsilon}$)。

牛顿势

$$\mathcal{H}(\boldsymbol{p},\boldsymbol{q})=\frac{1}{2m}\boldsymbol{p}^2-\frac{km}{|\boldsymbol{q}|}$$

在区域内 $G\neq 0$,$E_0(G)=-k^2m^3/2G^2<E<0$,$|G|<\sqrt{k^2m^3/(-2E)}$ 内是可积的。依循上节的步骤,可以找出积分坐标,并且会发现可积运动在一个焦点之一落在吸引中心 S 的椭圆上展开,从而运动是周期的,因此不是非等时的。但是,通过式[29]~[31]([39])构造正则坐标的程序同样有效,给出正则坐标(L',λ',G',γ')。为了得到容易诠释的作用量-角变量,可对(L',λ',G',γ')(用刚才介绍的程序构造)做一次平凡的正则变换,即令 $L=L'+G'$,$G=G'$,$\lambda=\lambda'$,$\gamma=\gamma'-\lambda'$,则

(1)λ(平均近点角)是点 P 从近心点到其当前位置所需的时间乘以 2π(以周期为单位);

(2)L(作用量)本质上就是能量 $E=-k^2m^3/2L^2$;

(3)G(角动量)[①];

(4)γ(沿长轴)是一固定轴和椭圆主轴(方向为从椭圆 O 的中心到吸引中心 S)之间的夹角。

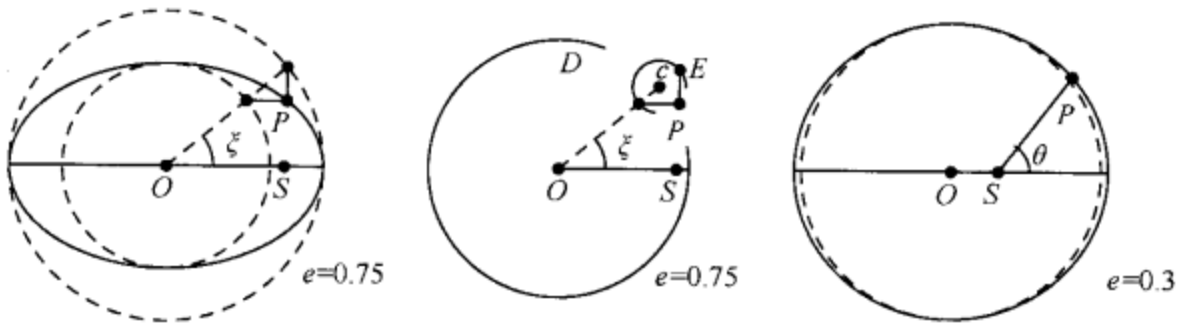

图 2　在小圆 E 上运动的 P 的偏近点角和真偏心角,小圆 E 的中心在 C 点且在圆 D 上运动,而图 D 处于包含开普勒椭圆的两个同心圆的半道上,这里 c 相对于轴 OS 的偏近点角是 ξ。圆 D 相对于 S 是偏心的,因此时至今日 ξ 一直被称为偏近点角,在古代词汇中,圆 D 被称为均轮圆(偏心圆是托勒密引入天文学的)。P 在其上运动的小圆 E 在古代词汇中称为本轮。均轮和本轮上的运动是同步的(即它们的周期相同);开普勒发现他的关键的预设,均轮上的角速度和 P 与 S 之间距离成反比(即 $\rho\dot{\xi}=$常数),意味着同时性和轨道的形状为焦点在 S 上的椭圆。后一定律等价于 $\rho^2\dot{\theta}=$常数(因为 $a\dot{\xi}=\rho\dot{\theta}$)。偏心率很小的椭圆很难同圆区分。

① 语法上说不过去,但原文如此——译者注。

椭圆的偏心率为 e,$G=\pm L\sqrt{1-e^2}$。椭圆的方程为 $\rho=a(1-e\cos\xi)$,ξ 是(见图 2)偏近点角,$a=L^2/km^2$ 是半长轴,ρ 是到吸引中心 S 的距离。

最后,偏近点角 ξ,平均近点角 λ,真近点角 θ(后者是极角),以及 SP 的时间 t 之间关系由开普勒方程给出:

$$\left.\begin{aligned}&\lambda=\xi-e\sin\xi\\&(1-e\cos\xi)(1+e\cos\theta)=1-e^2\\&\lambda=(1-e^2)^{3/2}\int_0^{\theta}\frac{\mathrm{d}\theta'}{(1+e\cos\theta')^2}\\&\frac{\rho}{a}=\frac{1-e^2}{1+e\cos\theta}\end{aligned}\right\}\qquad[41]$$

而真近点角和平均近点角之间的关系的逆有如下形式:

$$\left.\begin{aligned}&\xi=\lambda+g_\lambda\\&\theta=\lambda+f_\lambda\Rightarrow\frac{\rho}{a}=\frac{1-e^2}{1+e\cos(\lambda+f_\lambda)}\end{aligned}\right\}\qquad[42]$$

这里,$g_\lambda=g(e\sin\lambda,e\cos\lambda)$,$f_\lambda=f(e\sin\lambda,e\cos\lambda)$,而 $g(x,y)$,$f(x,y)$ 是 $|x|$,$|y|<1$ 上合适的解析函数。进一步,$g(x,y)=x(1+y+\cdots)$,$f(x,y)=2x\left(1+\frac{5}{4}y+\cdots\right)$,且省略号表示二阶项或 x,y 高阶项且仅含 x 的偶次幂。

欲知更多的细节,读者可参阅 Landau,Lifshitz(1976) 和 Gallavotti(1983)。

刚体

另一个基本的可积系统是不受引力作用的绕固定点 O 运动的刚体。它可以自然地用欧拉角 θ_0,φ_0,ψ_0(见图 3),及其导数 $\dot\theta_0$,$\dot\varphi_0$,$\dot\psi_0$,来描述。

令 $\boldsymbol{I}_1$,$\boldsymbol{I}_2$,$\boldsymbol{I}_3$ 为沿单位矢量 $\boldsymbol{i}_1$,$\boldsymbol{i}_2$,$\boldsymbol{i}_3$ 为主轴的 3 个主转动惯量。转动惯量和主轴分别是 3×3 惯量矩阵 $\mathcal{I}$ 的特征值和本征矢量。惯量矩阵定义为 $\mathcal{I}_{hk}=\sum_{i=1}^{n}m_i(\boldsymbol{x}_i)_h(\boldsymbol{x}_i)_k$,其中,$h,k=1,2,3$,而 $\boldsymbol{x}_i$ 是第 i 个粒子在以 O 为原点的、所有粒子在其中都静止的坐标系中的位置。这种随刚体一起运动坐标系的存在是刚性约束的结果。由主轴构成的坐标系同样是随刚体一起运动的,即在坐标系 $(O;\boldsymbol{i}_1,\boldsymbol{i}_2,\boldsymbol{i}_3)$ 中,粒子都是静止的。

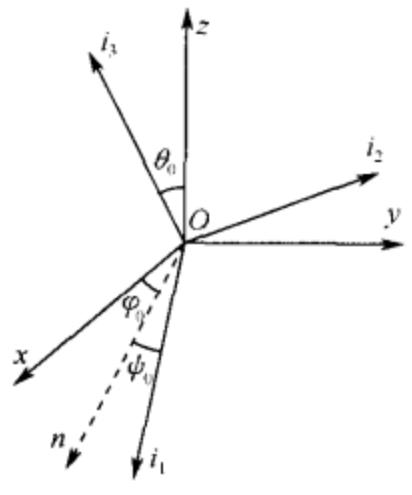

图 3 随刚体一起运动的坐标轴 $\boldsymbol{i}_1$,$\boldsymbol{i}_2$,$\boldsymbol{i}_3$ 同空间固定的坐标轴 $\boldsymbol{x}$,$\boldsymbol{y}$,$\boldsymbol{z}$ 之间的欧拉角,方向 $\boldsymbol{n}$ 是节线,即平面 $\boldsymbol{x}$,$\boldsymbol{y}$ 和平面 $\boldsymbol{i}_1$,$\boldsymbol{i}_2$ 的交叉线。

拉格朗日量就是动能,这里假设刚性约束是理想的(即如在“运动方程的拉格朗日和哈密顿形式”一节中所述的那样,由有心内力在无限刚性极限下所达成的那样)。刚体的角速度定义为

$$\boldsymbol{\omega}=\dot\theta_0\boldsymbol{n}+\dot\varphi_0\boldsymbol{z}+\dot\psi_0\boldsymbol{i}_3\qquad[43]$$

表明无限小运动由 3 个欧拉角的变化构成,因此它必定是绕轴 $\boldsymbol{n}$,$\boldsymbol{z}$,$\boldsymbol{i}_3$ 的且速率分别为 $\dot\theta_0$,$\dot\varphi_0$,$\dot\psi_0$ 的运动,如图 3 所示。

令$(\omega_1,\omega_2,\omega_3)$为$\boldsymbol{\omega}$沿主轴$(\boldsymbol{i}_1,\boldsymbol{i}_2,\boldsymbol{i}_3)$的分量,为简单起见,经常把这3个主轴称为**1,2,3**。可以验证绕支点O的角动量$\boldsymbol{M}$,以及动能K是:

$$\left.\begin{aligned} M &= I_1\omega_1\boldsymbol{i}_1 + I_2\omega_2\boldsymbol{i}_3 + I_3\omega_3\boldsymbol{i}_3 \\ K &= \frac{1}{2}(I_1\omega_1^2 + I_2\omega_2^2 + I_3\omega_3^2) \end{aligned}\right\} \qquad [44]$$

且为运动常数。由图3可得$\omega_1=\dot\theta_0\cos\psi_0+\dot\varphi_0\sin\theta_0\sin\psi_0$,$\omega_2=-\dot\theta_0\sin\psi_0+\dot\varphi_0\sin\theta_0\cos\psi_0$,$\omega_3=\dot\varphi_0\cos\theta_0+\dot\psi_0$,所以拉格朗日量为

$$\begin{aligned} L \overset{\text{def}}{=}& \frac{1}{2}I_1(\dot\theta_0\cos\psi_0+\dot\varphi_0\sin\theta_0\sin\psi_0)^2 \\ &+\frac{1}{2}I_2(-\dot\theta_0\sin\psi_0+\dot\varphi_0\sin\theta_0\cos\psi_0)^2 \\ &+\frac{1}{2}I_3(\dot\varphi_0\cos\theta_0+\dot\psi_0)^2 \end{aligned} \qquad [45]$$

角动量守恒并不意味分量ω是常数,因为$(\boldsymbol{i}_1,\boldsymbol{i}_2,\boldsymbol{i}_3)$也是根据下式随时间变化的:

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{i}_j = \boldsymbol{\omega}\wedge\boldsymbol{i}_j,\quad j=1,2,3$$

由此,根据式[44]的第一式,引入表示$\boldsymbol{I\omega}=(\boldsymbol{I}_1\omega_1,\boldsymbol{I}_2\omega_2,\boldsymbol{I}_3\omega_3)$,$\dot{\boldsymbol{M}}=0$变成了欧拉方程$\boldsymbol{I}\dot{\boldsymbol{\omega}}+\boldsymbol{\omega}\wedge\boldsymbol{I\omega}$,或者

$$\left.\begin{aligned} \boldsymbol{I}_1\dot\omega_1 &= (\boldsymbol{I}_2-\boldsymbol{I}_3)\omega_2\omega_3 \\ \boldsymbol{I}_2\dot\omega_2 &= (\boldsymbol{I}_3-\boldsymbol{I}_1)\omega_3\omega_1 \\ \boldsymbol{I}_3\dot\omega_3 &= (\boldsymbol{I}_1-\boldsymbol{I}_2)\omega_1\omega_2 \end{aligned}\right\} \qquad [46]$$

这些可以和式[44]中的守恒量一同考虑。

因为角动量是守恒的,可以方便地引入带固定轴$\boldsymbol{x}_0,\boldsymbol{y}_0,\boldsymbol{z}_0$的**实验室坐标系**$(O;x_0,y_0,z_0)$(见图4):

(1)动量坐标系$(O;x,y,z)$的轴固定,但z轴沿$\boldsymbol{M}$方向,x轴和平面x_0-y_0与平面$x-y$的节线重合(与$\boldsymbol{M}$正交)。因此x,y,z由$(O;x,y,z)$在$(O;x_0,y_0,z_0)$中的两个欧拉角ζ,γ决定。

(2)随动的坐标系$(O;1,2,3)$是固定在刚体上的,其轴平行于刚体的主轴且具有单位矢量$\boldsymbol{i}_1,\boldsymbol{i}_2,\boldsymbol{i}_3$。此坐标系由3个欧拉角$\theta_0,\varphi_0,\psi_0$决定。

(3)坐标系$(O;\boldsymbol{1},\boldsymbol{2},\boldsymbol{3})$关于坐标系$(O;x,y,z)$的3个欧拉角可表为$\theta,\varphi,\psi$。

(4)G为总角动量:$G^2=\sum_j\boldsymbol{I}_j^2\omega_j^2$。

(5)M_3为沿z_0方向的角动量,$\boldsymbol{M}_3=G\cos\zeta$。

(6)L为$\boldsymbol{M}$在轴3方向上的投影,$L=G\cos\theta$。

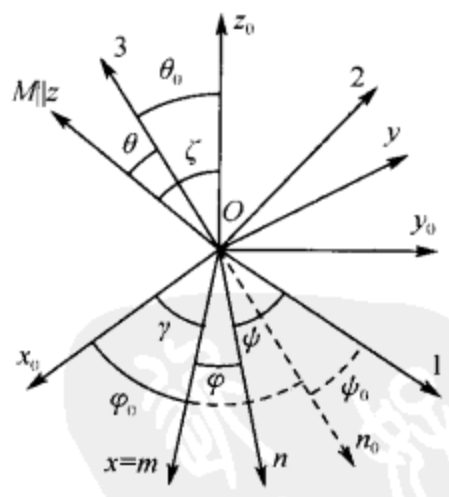

图4　实验室坐标系,角动量坐标系和随刚体运动的坐标系(及Deprit角)[①]。

①André Deprit(1926～2006),美国天体物理学教授,擅长符号计算。当前中文书籍中少见把这套角标记称为Deprit角——译者注。

量 $G,M_3,L,\varphi,\gamma,\psi$ 决定 $\theta_0,\varphi_0,\psi_0$ 和 $\dot{\theta}_0,\dot{\varphi}_0,\dot{\psi}_0$,或 $\theta_0,\varphi_0,\psi_0$ 的共轭变量 $p_{\theta_0},p_{\varphi_0},p_{\psi_0}$。详细讨论如下。

考虑图 4,角 ζ,γ 决定了 $\boldsymbol{M}$ 方向和节线 $\boldsymbol{m}$,它们分别是与角动量联系坐标系的 z 轴及 x 轴在固定坐标系 $(O;x_0,y_0,z_0)$ 中的位置;而角 θ,φ,ψ 决定了随动的坐标系在坐标系 $(O;x,y,z)$ 中的位置①,当然也决定了在坐标系 $(O;x_0,y_0,z_0)$ 中的位置,即角 $\theta_0,\varphi_0,\psi_0$。从这一点和总角动量 $\boldsymbol{G}$ 可以导出 $\boldsymbol{\omega}$,因为

$$\cos\theta=\frac{\boldsymbol{I}_3\omega_3}{G},\tan\psi=\frac{\boldsymbol{I}_2\omega_2}{\boldsymbol{I}_1\omega_1}$$

$$\omega_2^2=\boldsymbol{I}_2^{-2}(G^2-\boldsymbol{I}_1^2\omega_1^2-\boldsymbol{I}_3^2\omega_3^2) \qquad [47]$$

再由式[43]可得到 $\dot{\theta}_0,\dot{\varphi}_0,\dot{\psi}_0$。

式[45]中的拉格朗日量直接给出了(用角 $\theta_0,\varphi_0,\psi_0$ 表达 $\boldsymbol{\omega}$,即 $\boldsymbol{n},\boldsymbol{z},\boldsymbol{i}_3$)$\theta_0,\varphi_0,\psi_0$ 共轭变量 $p_{\theta_0},p_{\varphi_0},p_{\psi_0}$ 的表达式:

$$p_{\theta_0}=\boldsymbol{M}\cdot\boldsymbol{n}_0,\qquad p_{\varphi_0}=\boldsymbol{M}\cdot\boldsymbol{z}_0,\qquad p_{\psi_0}=\boldsymbol{M}\cdot\boldsymbol{i}_3 \qquad [48]$$

并在原则上可以进一步计算哈密顿量。

然而,因为有下面的一个重要性质(Deprit),没必要进行这样的计算。这个性质可以利用式[48]和初等球面三角恒等式得到,

$$M_3\mathrm{d}\gamma+G\mathrm{d}\varphi+L\mathrm{d}\psi=p_{\varphi_0}\mathrm{d}\varphi_0+p_{\psi_0}\mathrm{d}\psi_0+p_{\theta_0}\mathrm{d}\theta_0 \qquad [49]$$

它意味着映射$((M_3,\gamma),(L,\psi),(G,\varphi))\leftrightarrow((p_{\theta_0},\theta_0),(p_{\varphi_0},\varphi_0),(p_{\psi_0},\psi_0))$是正则映射。在新坐标系里,动能,也就是哈密顿量的表达式为

$$K=\frac{1}{2}\left[\frac{L^2}{\boldsymbol{I}_3}+(G^2-L^2)\left(\frac{\sin^2\psi}{\boldsymbol{I}_1}+\frac{\cos^2\psi}{\boldsymbol{I}_2}\right)\right] \qquad [50]$$

这再一次表明 G,M_3 是运动常数,而 L,ψ 是由二次型决定的变量,因为由 ψ 的哈密顿方程,加上能量守恒,可得到

$$\dot{\psi}=\pm\left(\frac{1}{\boldsymbol{I}_3}-\frac{\sin^2\psi}{\boldsymbol{I}_1}-\frac{\cos^2\psi}{\boldsymbol{I}_2}\right)\times\sqrt{\frac{2E-G^2\left(\frac{\sin^2\psi}{\boldsymbol{I}_1}+\frac{\cos^2\psi}{\boldsymbol{I}_2}\right)}{\frac{1}{\boldsymbol{I}_3}-\frac{\sin^2\psi}{\boldsymbol{I}_1}-\frac{\cos^2\psi}{\boldsymbol{I}_2}}} \qquad [51]$$

在可积性区域内,运动是周期性的,周期为 $T_L(E,G)$。一旦 $\psi(t)$ 被决定了,φ 的哈密顿方程可导出二次型

$$\dot{\varphi}=\left(\frac{\sin^2\psi(t)}{\boldsymbol{I}_1}+\frac{\cos^2\psi(t)}{\boldsymbol{I}_2}\right)G, \qquad [52]$$

它决定了另一个周期为 $T_G(E,G)$ 的周期性运动。γ, M_3 是常数,因此运动是在相空间的三维不变圆环面 $\mathcal{T}_{E,G,M_3}$ 上进行的,且每个圆环面总是可以分叶成由 γ 角加以参数化的二维圆环面的叶状结构,γ 是个常量(可由式[50]得到,因为 K 不依赖于 M_3),而二维圆环面又可以分叶为一维不变圆环面的叶状结构,即周期运动轨道,其对应的 E,G 使得 $T_L(E,G)/T_G(E,G)$ 是有理数。

注意到如果 $\boldsymbol{I}_1=\boldsymbol{I}_2=\boldsymbol{I}$,上述分析将大大简化。进一步,如果引力 g 作用在系统上,哈

① 此处原文误把$(O;x,y,z)$也称为固定坐标系了——译者注。

密顿量的变化只是添加了势能$-mgz$,z是质心的高度。如果质心在轴$\boldsymbol{i}_3$上,$z=h\cos\theta_0$,h是质心到原点O的距离(见图4),因为有$\cos\theta_0=\cos\theta\cos\zeta-\sin\theta\sin\zeta\cos\varphi$,哈密顿量变成$\mathcal{H}=K-mgh\cos\theta_0$,或者

$$\mathcal{H}=\frac{G^2}{2\boldsymbol{I}_3}+\frac{G^2-L^2}{2\boldsymbol{I}}-mgh\left(\frac{M_3L}{G^2}-\left(1-\frac{M_3^2}{G^2}\right)^{1/2}\times\left(1-\frac{L^2}{G^2}\right)^{1/2}\cos\varphi\right) \qquad [53]$$

这样系统又是在相空间合适的区域内是二次型可积的(和前例比较,ψ和φ的角色互换了)。这样的系统称为**拉格朗日陀螺**。

一个略有难度的可积情形是这样的,惯量$\boldsymbol{I}_1=\boldsymbol{I}_2=2\boldsymbol{I}_3$,质心在$\boldsymbol{i}_1-\boldsymbol{i}_2$平面内(而非在轴$\boldsymbol{i}_3$上),除了来自支点$O$的约束力之外,只有引力作用。这样的系统称为**科瓦列夫斯卡娅陀螺**。

欲知更多的细节,读者可参阅Gallavotti(1983)。

其他二次型

一个有趣的经典可积模型是被两个等质量的中心所吸引的质点,或在一般的旋转椭球面上的理想约束运动的质点。

近年发现了一些新的可积系统,并且在从群论(可积系统同对称性有密切的关联)到偏微分方程方面取得了大量的新进展。

可以方便地把可积性的概念扩展为:一个系统在相空间的区域W上是可积的,如果

(1) 有坐标变换$(\boldsymbol{p},\boldsymbol{q})\in W\leftrightarrow\{\boldsymbol{A},\boldsymbol{\alpha},\boldsymbol{Y},y\}\in(U\times\mathbb{T}^l)\times(V\times\mathbb{R}^m)$,其中$U\subset\mathbb{R}^m$和$V\subset\mathbb{R}^l$是开集,$l+m\geqslant 1$;

(2) $\boldsymbol{A},\boldsymbol{Y}$是运动常量,而其他坐标是"线性"变化的

$$(\boldsymbol{\alpha},y)\rightarrow(\boldsymbol{\alpha}+\boldsymbol{\omega}(\boldsymbol{A},\boldsymbol{Y})t,y+v(\boldsymbol{A},\boldsymbol{Y})t) \qquad [54]$$

这里的$\boldsymbol{\omega}(\boldsymbol{A},\boldsymbol{Y})$,$v(\boldsymbol{A},\boldsymbol{Y})$是光滑函数。

在新的意义上,前述章节研究的系统在更宽泛的区域内是可积的(基本上是在整个相空间内可积,例外只是一些在低维曲面上构成体积为零之集合的点集)。这个概念也是方便应用的,因为它允许我们说甚至自由粒子体系也是可积的。

在新的意义下,两个值得注意的可积的系统分别是称为**Toda格子**(Kruskal,Zabusky)和**Calogero格子**(Calogero,Moser)的哈密顿系统。如果$(\boldsymbol{p}_i,\boldsymbol{q}_i)\in\mathbb{R}^2$,它们的哈密顿量为

$$\left.\begin{aligned}\mathcal{H}_{\mathrm{T}}(p,q)&=\frac{1}{2m}\sum_{i=1}^{n}p_i^2+\sum_{i=1}^{n-1}g\mathrm{e}^{-\kappa(q_{i+1}-q_i)}\\ \mathcal{H}_{\mathrm{C}}(p,q)&=\frac{1}{2m}\sum_{i=1}^{n}p_i^2+\sum_{i<j}^{n}\frac{g}{(q_i-q_j)^2}+\frac{1}{2}\sum_{i=1}^{n}m\omega^2q_i^2\end{aligned}\right\} \qquad [55]$$

这里$m>0$,$k,\omega,g\geqslant 0$,描述的是在一条线上的n个相互作用粒子的运动。

上述系统的积分方法同样是先找到运动常数,然后找出适当的二次型。运动常数可由**Lax**对的方法找到。有一对自伴的$n\times n$矩阵$M(\boldsymbol{p},\boldsymbol{q})$,$N(\boldsymbol{p},\boldsymbol{q})$使得运动方程变成

$$\frac{\mathrm{d}}{\mathrm{d}t}M(\boldsymbol{p},\boldsymbol{q})=i[M(\boldsymbol{p},\boldsymbol{q}),N(\boldsymbol{p},\boldsymbol{q})],\ i=\sqrt{-1} \qquad [56]$$

这意味着$\boldsymbol{M}(t)=\boldsymbol{U}(t)\boldsymbol{M}(0)\boldsymbol{U}(t)^{-1}$,而$\boldsymbol{U}(t)$是一个幺正矩阵。当方程能写成上述形式的

时候,显然矩阵 $\boldsymbol{M}_0=\boldsymbol{M}_0(\boldsymbol{p}_0,\boldsymbol{q}_0)$ 的 n 个特征值是运动常数。在合适的情况下(例如,在具有 $\omega>0$ 的 Calogero 格子中),能够进一步找出正则的作用量-角坐标。这个任务由于 n 的随意性而显得很困难,但却是可能的。

关于 Calogero 格子($\omega=0, g=m=1$)的 Lax 对是

$$\boldsymbol{M}_{hh}=p_h,\boldsymbol{N}_{hh}=0$$

$$\boldsymbol{M}_{hk}=\frac{i}{(q_h-q_k)},\boldsymbol{N}_{hk}=\frac{1}{(q_h-q_k)^2},^{①}\ h\neq k \qquad [57]$$

而关于 Toda 格子$\left(m=g=\frac{1}{2}\kappa=1\right)$,$\boldsymbol{M},\boldsymbol{N}$ 的非零矩阵元为

$$\boldsymbol{M}_{hh}=p_h,\boldsymbol{M}_{h,h+1}=\boldsymbol{M}_{h+1,h}=\mathrm{e}^{-(q_h-q_{h+1})}$$

$$\boldsymbol{N}_{h,h+1}=-\boldsymbol{N}_{h+1,h}=i\mathrm{e}^{-(q_h-q_{h+1})} \qquad [58]$$

可以先在 $n=2$ 的情形试着加以验证。

另一个可积系统(Sutherland)是

$$\mathcal{H}_S(\boldsymbol{p},\boldsymbol{q})=\frac{1}{2m}\sum_{i=k}^{n}p_k^2+\sum_{h<k}^{n}\frac{g}{\sinh^2(q_h-q_k)} \qquad [59]$$

其 Lax 对和 Calogero 格子的 Lax 对相联系。

取合适的极限 $n\to\infty$,其他参数以合适的速度趋于 0 或∞,可以得到一些微分方程——比如 KdV 方程或非线性薛定谔方程的可积性证明。

如"导论"一节中所言,连续群下的对称性意味着运动常数的存在。很自然会想到,一个力学体系的可积性反映出足够的对称性保证有多达自由度 n 那么多个运动常数,独立的或内卷的存在。

这个陈述实际上总是为真的,在非等时情况下,这在某些方面看来甚至是无需多言的。在区域 W 内的可积性意味着存在正则作用量-角坐标$(\boldsymbol{A},\boldsymbol{\alpha})$(见"准周期性与可积性"一节),哈密顿量只依赖于 $\boldsymbol{A}$:因此它对 W 的限制相对于角变量平移的连续交换群 T^n 的作用是不变的。作用量可看作是运动常数,至少在非等时情况下(哈密顿表述和拉格朗日表述等价的),其存在性由 Noether 定理保证。

不同寻常的是,在认识到可积性之前,人们就知道存在这样的对称性:在大多数人们感兴趣的情况下,系统要么不存在明显的对称性,要么对称性看起来和群 T^n 无关,但它却暗示存在足够多的可积性所要求的独立的运动常数。因此,非平凡的可积系统拥有 T^n 下的"隐"对称性,刚体就是个例子。

然而,一个哈密顿量 H 的对称性暗含可积性常常也意味着部分的等时性,也就是说独立的频率数要少于 n(见"准周期性与可积性"一节)。即便在这些情况下,常常存在从原来的坐标$(\boldsymbol{p},\boldsymbol{q})$到积分变量$(\boldsymbol{A},\boldsymbol{\alpha})$的映射,$\boldsymbol{A}$ 是运动常数,而 $\boldsymbol{\alpha}$ 是谱为 $\boldsymbol{\omega}(\boldsymbol{A})$(为某个只依赖于 $\boldsymbol{A}$ 坐标的函数 $h(\boldsymbol{A})$的梯度$\partial_A h(\boldsymbol{A})$)的匀速转动角(有些也是常数)。但是映射不是正则的。这样的系统在下述意义中被称为双哈密顿的:可以在相互间不能够通过正则变换联系的两个正则坐标系中,用两个哈密顿函数 H 和 $H'\equiv h$ 来描述其运动。H 和 H' 在相应的坐标系中产生同样的运动(刚才的变量改变有时被称为"关于 H,H' 对是正则

① 原文中有笔误 —— 译者注。

的",而在"相空间坐标的正则变换"一节里考虑的变换被称为完全正则的)。

欲知更多的细节,读者可参阅 CalogeroI,Degasperis (1982)。

通有不可积性

人们很自然地想证明,一个和可积系统很"接近"的系统其运动的性质也非常接近是准周期的。确实是这样,但是是以一种非常微妙的方式。存在的问题可以很容易地从非等时可积系统扰动的例子中看到。

假设某系统在相空间的区域 W 上是可积的,用积分作用量-角变量表示,区域有标准形式 $U\times\mathbb{T}^l$,其哈密顿量 $h(\boldsymbol{A})$ 的梯度为 $\boldsymbol{\omega}(\boldsymbol{A})=\partial_A h(\boldsymbol{A})$。如果作用力为一个光滑的势所扰动,则新系统在原来的坐标系中可以用类似

$$H_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha}) = h(\boldsymbol{A}) + \varepsilon f(\boldsymbol{A},\boldsymbol{\alpha}) \qquad [60]$$

的哈密顿量描述,h,f 是 $\boldsymbol{A},\boldsymbol{\alpha}$ 的解析函数。

如果系统的行为真的如未扰动的系统那样,它一定有形如 $F_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha})$ 的 l 个运动常数,且 $F_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha})$ 是在 $\varepsilon=0$ 附近关于 ε 解析的,一致的,即关于变量 $\boldsymbol{\alpha}$ 单值的(即是说周期的)。但是,下面的定理(Poincaré)却表明很少是这样的。

定理 1　如果矩阵 $\partial^2_{AA}h(\boldsymbol{A})$ 的秩 $\geqslant 2$,则式[60]中的哈密顿量"通有地"(这是直观的描述,确切意义见下)不可以被这样的正则变换 $C_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha})$ 进行积分,它

(i)当 $\varepsilon\to 0$ 时退化为全等变换;

(ii)是关于 $\varepsilon=0$ 附近的 ε,关于 $(\boldsymbol{A},\boldsymbol{\alpha})\in U'\times\mathbb{T}^l$ ($U'\subset U$ 是开集)是解析的。

而且,除了 H_ε 本身以外,不存在其他的对 $\varepsilon=0$ 附近的 ε 和开区域 $U'\times\mathbb{T}^l$ 上的 $(\boldsymbol{A},\boldsymbol{\alpha})$ 定义的一致的运动常数 $F_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha})$。

在(i)和(ii) 意义下的可积性称为解析可积性,它也是关于这一性质所能给出的最强的(也是最质朴的)表述。

定理的第一部分,即关于(i)和(ii)的论述成立是因为,在假设了可积性后,积分映射的生成函数就有形式 $\boldsymbol{A}'\cdot\boldsymbol{\alpha}+\Phi_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha})$,而 Φ 关于 ε 有级数展开 $\Phi_\varepsilon=\varepsilon\Phi^1+\varepsilon^2\Phi^2+\cdots$。因此,$\Phi^1$ 必需满足

$$\boldsymbol{\omega}(\boldsymbol{A}')\cdot\partial_a\Phi^1(\boldsymbol{A}',\boldsymbol{\alpha}) + f(\boldsymbol{A}',\boldsymbol{\alpha}) = \bar{f}(\boldsymbol{A}') \qquad [61]$$

这里 $\bar{f}(\boldsymbol{A}')$ 只依赖于 $\boldsymbol{A}'$(两侧都对 $\boldsymbol{\alpha}$ 积分,可见 $\bar{f}(\boldsymbol{A}')$ 必须等同于 $f(\boldsymbol{A}',\boldsymbol{\alpha})$ 对 $\boldsymbol{\alpha}$ 的平均)。

这意味着傅里叶变换 $f_v(\boldsymbol{A})$,$v\in\mathbb{Z}^l$,应该满足

$$f_v(\boldsymbol{A}')=0 \quad \text{如果 } \boldsymbol{\omega}(\boldsymbol{A}')\cdot\boldsymbol{v}=0,\boldsymbol{v}\neq 0 \qquad [62]$$

这等价于存在 $\tilde{f}_v(\boldsymbol{A}')$,使得对 $\boldsymbol{v}\neq 0$ 有 $f_v(\boldsymbol{A})=\boldsymbol{\omega}(\boldsymbol{A}').\boldsymbol{v}\tilde{f}_v(\boldsymbol{A}')$。但是,因为 $\boldsymbol{\omega}(\boldsymbol{A})$ 和 $f(\boldsymbol{A},\boldsymbol{\alpha})$ 之间没有关系,这个性质"通有地"就不成立。意思是不论离满足式[62]的 f 有多近,也不论"近"是如何定义(例如,就度量 $\|f-g\|=\sum_v|f_v(\boldsymbol{A})-g_v(\boldsymbol{A})|$ 而言)的,都有不满足它的另一个 f。这是因为矩阵 $\partial^2_{AA}h(A)$ 的秩比 1 高,且 $\boldsymbol{\omega}(\boldsymbol{A})$ 是在至少是二维的曲面上变化,所以对某些 $v\neq 0$,$\boldsymbol{\omega}\cdot\boldsymbol{v}=0$ 肯定是可能的,而 $f_v(\boldsymbol{A})$ 一般不会为零,所以 Φ^1 不存在,因此 Φ_ε 也就不存在。

也就是说,函数 f 附近总有另一个函数 f',对某些 v,违背式[62]。当然,这取决于

"近"的含义。但本质上,在函数 f 的空间上引入的任何拓扑都会使得上述陈述是正确的:比如,若两个函数之间的距离是由 $\sum_v \sup_{A\in U}|f_v(\boldsymbol{A})-g_v(\boldsymbol{A})|$ 和 $\sup_{A,\alpha}|f(\boldsymbol{A},\boldsymbol{\alpha})-g(\boldsymbol{A},\boldsymbol{\alpha})|$ 定义的。

关于上述定理前面的陈述,其背后的思想本质上是相同的。为简单起见,考虑非等时情形下矩阵 $\partial^2_{AA}h(\boldsymbol{A})$ 有最大秩 l,即矩阵值 $\det\partial^2_{AA}h(\boldsymbol{A})$ 不为零。非等时性意味着对所有的 $v\neq 0$,在 $\boldsymbol{A}$ 稠集上 $\boldsymbol{\omega}(\boldsymbol{A})\cdot v\neq 0$。下面的分析中会多次用到这个性质。

令 $B(\epsilon,\boldsymbol{A},\boldsymbol{\alpha})$ 为一"一致"的运动常数,意思即它是单值的,在非单连通的区域 $U\times\Omega'$ 上是解析的,且对小的 ϵ 有

$$B(\epsilon,\boldsymbol{A},\boldsymbol{\alpha})=B_0(\boldsymbol{A},\boldsymbol{\alpha})+\epsilon B_1(\boldsymbol{A},\boldsymbol{\alpha})+\epsilon^2 B_2(\boldsymbol{A},\boldsymbol{\alpha})+\cdots \qquad [63]$$

B 是运动常数的条件可以根据它对 ϵ 的展开一阶一阶地写出,前两阶是

$$\left.\begin{aligned}&\boldsymbol{\omega}(\boldsymbol{A})\cdot\partial_{\boldsymbol{\alpha}}B_0(\boldsymbol{A},\boldsymbol{\alpha})=0\\&\partial_{\boldsymbol{A}}f(\boldsymbol{A},\boldsymbol{\alpha})\cdot\partial_{\boldsymbol{\alpha}}B_0(\boldsymbol{A},\boldsymbol{\alpha})-\partial_{\boldsymbol{\alpha}}f(\boldsymbol{A},\boldsymbol{\alpha})\cdot\partial_{\boldsymbol{A}}B_0(\boldsymbol{A},\boldsymbol{\alpha})+\boldsymbol{\omega}(\boldsymbol{A})\cdot\partial_{\boldsymbol{\alpha}}B_1(\boldsymbol{A},\boldsymbol{\alpha})=0\end{aligned}\right\} \qquad [64]$$

上述的两个关系和非等时性意味着:(1)B_0 必须仅是 $\boldsymbol{A}$ 的函数,(2)$\boldsymbol{\omega}(\boldsymbol{A})\cdot v$ 和 $\partial_{\boldsymbol{A}}B_0(\boldsymbol{A})\cdot v$ 对所有的 v 同时为零。因此,B_0 的梯度必须同 $\boldsymbol{\omega}(\boldsymbol{A})$,即 $h(\boldsymbol{A})$ 的梯度 $\partial_{\boldsymbol{A}}B_0(\boldsymbol{A})=\lambda(\boldsymbol{A})\partial_{\boldsymbol{A}}h(\boldsymbol{A})$,成正比。所以通有地(因为非等时性)一定有 B_0 是通过 $h(\boldsymbol{A})$ 而依赖于 $\boldsymbol{A}$ 的,即对于某个 F,$B_0(\boldsymbol{A})=F(h(\boldsymbol{A}))$。

带着这些新信息,再考察式[64]的第二式,可知在固定点 $\boldsymbol{A}$,B_1 在 $\boldsymbol{\omega}(\boldsymbol{A})$ 方向上的 $\boldsymbol{\alpha}$ 导数等于 $F'(h(\boldsymbol{A}))$ 乘上 f 的 $\boldsymbol{\alpha}$ 导数,即 $B_1(A,\alpha)=f(\boldsymbol{A},\boldsymbol{\alpha})F'(h(\boldsymbol{A}))+C_1(\boldsymbol{A})$。

总结:运动常数 B 被写为 $B(\boldsymbol{A},\boldsymbol{\alpha})=F(h(\boldsymbol{A}))+\epsilon F'(h(\boldsymbol{A}))f(\boldsymbol{A},\alpha)+\epsilon C_1(\boldsymbol{A})+\epsilon^2 B_2+\cdots$,它等价于 $B(\boldsymbol{A},\boldsymbol{\alpha})=F(\mathcal{H}_\epsilon)+\epsilon(B_0'+\epsilon B_1'+\cdots)$,因此 $B_0'+\epsilon B_1'+\cdots$ 是另一个解析的运动常数。重复上述讨论,$B_0'+\epsilon B_1'+\cdots$ 也必须有形式 $F_1(\mathcal{H}_\epsilon)+\epsilon(B_0''+\epsilon B_1''+\cdots)$;结论是

$$B=F(\mathcal{H}_\epsilon)+\epsilon F_1(\mathcal{H}_\epsilon)+\epsilon^2 F_2(\mathcal{H}_\epsilon)+\cdots+\epsilon^n F_n(\mathcal{H}_\epsilon)+O(\epsilon^{n+1}) \qquad [65]$$

按照解析性,对某些 F_ϵ,$B=F_\epsilon(\mathcal{H}_\epsilon(\boldsymbol{A},\boldsymbol{\alpha}))$;因此,从属性上说所有的运动常数都是平凡的。

因此,一个接近可积系统的系统,其行为并不是如天真预期那样的。可是问题不是那么显而易见的,直到庞加莱证明了上述结果。因为在大多数应用中函数 f 只有有限多的傅里叶分量,或可以由具有这种性质的近似函数所替代,使得至少式[62]以及甚至一些像式[64]那样的高阶约束在作用量空间的开区域上都是有可能的。实际上,有意思的 $\boldsymbol{A}$ 的值被限制为那些只是对满足 $f_v=0$ 的"大"值的 v 才有 $\boldsymbol{\omega}(\boldsymbol{A})\cdot v=0$。不过,微扰系统的解析可积性的必要条件,即性质 $f_v(\boldsymbol{A})=(\boldsymbol{\omega}(\boldsymbol{A})\cdot v)f_v(\boldsymbol{A})$(或者可类比的高阶条件,如式[64]),对许多重要问题来说,如果不对 f 做近似,可以验证是不满足的。这样就出现了概念上的问题。

欲知更多的细节,读者可参阅 Poincaré(1987)。

扰动函数

对给定的问题,要沿着前述章节里的思路验证不存在非平凡的运动常数,有必要把势用未扰动的可积系统的作用量-角变量表述出来,而通常它们被用笛卡儿坐标给出为 $\epsilon V(\boldsymbol{x})$。

特别的,在非等时性假设不满足时(比较前一节),试图验证不存在非平凡的运动常数是会出问题的。通常,非等时性假设在二阶(或更高阶)上是满足的,不过,要表明这一点,关于扰动函数(用作用量-角坐标表述)之结构的更多信息是必要的。比如,当把扰动用三角多项式近似的时候,就必须知道扰动函数结构的更多信息,实际上在天体力学中这样做是常事。

如何给出作用量-角变量的显式表达本来就不是一件平凡的事,即使是在一些看起来简单的情形下它都会引起一些具有内在兴趣的问题。例如,对平面引力有心运动,开普勒方程 $\lambda=\xi-\epsilon\sin\xi$(见式[41]第一式)的解需要用 λ 表达 ξ(见式[42]第一式)。明显的,对小的 ϵ,变量 ξ 可以表示为 ϵ 的一个解析函数,但是,表达式的实际构造会导致一些问题。对小的 ϵ,下面介绍一个有趣的算法:

令 $h(\lambda)=\xi-\lambda$,则要解的方程(即式[41]第一式)为

$$h(\lambda)=\epsilon\sin(\lambda+h(\lambda))\equiv-\epsilon\frac{\partial c}{\partial\lambda}(\lambda+h(\lambda)) \qquad [66]$$

这里 $c(\lambda)=\cos\lambda$。函数 $\lambda\to h(\lambda)$ 应该关于 λ 是周期的,周期为 2π,关于小的 ϵ 和实的 λ 是解析的。如果 $h(\lambda)=\epsilon h^{(1)}+\epsilon^2 h^{(2)}+\cdots$,傅里叶变换 $h^{(k)}(\lambda)$ 满足递归关系

$$h_v^{(k)}=-\sum_{p=1}^{\infty}\frac{1}{p!}\sum_{\substack{k_1+\cdots+k_p=k-1\\ v_0+v_1+\cdots+v_p=v}}(iv_0)c_{v_0}(iv_0)^p\times\prod h_{v_j}^{(k_j)},\qquad k>1 \qquad [67]$$

c_v 是余弦函数的傅里叶变换 $\left(c_{\pm1}=\frac{1}{2};c_v=0,v\neq\pm1\right)$,$h_v{}^{(1)}=-ivc_v$。方程[67]是将式[66]右边项展开成 h 的级数,然后对两边做傅里叶变换,保留 ϵ 的 k 次幂项得到的。

按上述关系递推,如图 5 那样画出所有含 k 分枝(或"连线")的 θ 树,由取 k 个不同值的标签,k 个节点加以区分,对每个节点 v 附上一个谐波标签 $v_v=\pm1$。这样的树从一条连接点 r 和"第一个节点"v 的根线 vr(见图 5[①])开始,然后随意分岔(这样的树有时被称为"有根树")。

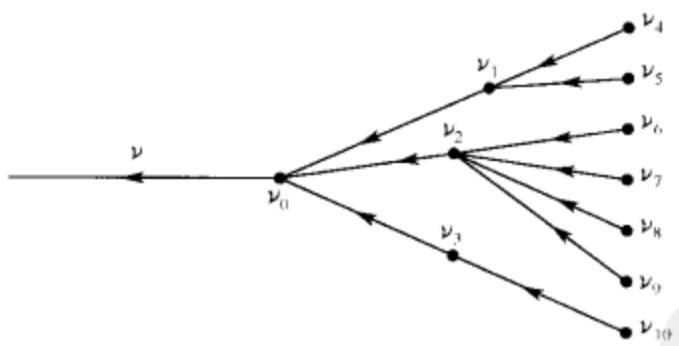

图 5　树图和标签。此图只包含一个简单的节点(3)。谐波项的标签紧挨着节点,区分不同"连线"的标签没有画出。

想像一棵从终点指向根 r(不可以当作节点考虑)的树,给定树上的一个节点 v,其紧邻的节点为 v'。如果 v 是根 r 前面的第一个节点,令 $v'=r,v_{v'}=1$。对每一个这样装饰了的树定义它的数值为

① 图 5 中未标记出 r——译者注。

$$\mathrm{Val}(\theta) = \frac{-i}{k!}\prod_{\text{lines } l=v'v}(v_{v'}v_v)\prod_{\text{nodes}}c_{v_v} \qquad [68]$$

且定义线 $l=v'v$ 上的流 $v(l)$ 为节点 v' 前面所有节点的谐波的和，$v(l)=\sum_{w\leqslant v}v_w$ ①。称 $v(\theta)$ 为根叉上的流，称 θ 的阶为节点(分枝)的数目。若树在对其分枝的长度做合适的尺度变换后　　分枝被钉扎在节点上(根总是固定在原点上)　　是重合的就认定是等同的，则

$$h_v^{(k)} = \sum_{\substack{\theta,v(\theta)=v\\ \mathrm{order}(\theta)=k}}\mathrm{Val}(\theta) \qquad [69]$$

如果删去树的谐波标签，树的数目是有限的，可估计其$\leqslant k!\,4^k$(因为区分"连线"的标签可以用多种方式添加到一个未标记的树上)。谐波标签(即 $v_v=\pm1$)可以 2^k 种方式加上，则每棵树的值的上限为$(1/k!)2^{-k}\left(\text{因为 } c_1=\frac{1}{2}\right)$。

因此，$\sum_v|h_v^{(k)}|\leqslant 4^k$ 给出了对 h 的 ϵ 级数展开的收敛半径上限的估计，为 0.25(如果用 k^{k-1} 代替 $4^k k!$，用有根树计数的 Cayley 公式计算，则可容易得出改进值为 0.3678)。$h^{(k)}(\psi)$的一个简单表达式(Lagrange)为

$$h^{(k)}(\psi) = \frac{1}{k!}\partial_\psi^{k-1}\sin^k\psi$$

(可从树表示直接得到)。h 级数真正的收敛半径(首先由拉普拉斯给出)可以从上面关于 h 的表达式(Rouché)得到，也可以直接从树表示得到，约为 0.6627。

可以找到更好的估计或对式[69]求和的更有效的方法。实际上，在对式[69]求和时，有许多重要的项抵消了。例如，谐波标签可以置于更强的约束下，即没有携带零流的连线，因为固定阶的且至少一条连线上的流为零的树，它们的值的和为零。

上述的展开可以用**部分求和**加以简化。为了下面的举例，我们称单进单出的节点(见图 5)为"简单"节点。所有的树图，若在连接两个非简单的节点的连线上有任何数目的简单节点，都可以去除。这可以通过对(剩余)树求值时用 $v_{v'}v_v/(1-\epsilon\cos\psi)$ 替代式[68]中的 $v_{v'}v_v$ 来实现，树的 θ 值(记为 $\mathrm{Val}(\theta)_\psi$)变成了 ψ 和 ϵ 的函数，式[69]被替换成

$$h(\psi) = \sum_{k=1}^{\cdots}\sum_{\substack{\theta,v(\theta)=v\\ \mathrm{order}(\theta)=k}}^{*}\epsilon^k e^{in\psi}\mathrm{Val}(\theta)_\psi \qquad [70]$$

这里 * 号的意思是树被置于不包含简单节点的强约束下。注意到上述的开普勒方程解的图表示含有强烈的量子场论用图表示量的痕迹，这里的树对应于**费曼图**，同节点相联系的因子为**耦合常数**，同连线相联系的因子为**传播子**，求和类比于**自能项的求和**，而前述的抵消可以同称为 **Ward 恒等式**的一类恒等式相联系。这样的类比不仅不是表面的，在许多关键的力学问题上会发现它是非常有用的，参见附录一。

同树的值相联系存在大量的恒等式，这一点早已为拉格朗日级数的**简单**形式以及更重要的导致

$$h(\psi) = \sum_{k=1}^{\cdots}\frac{(\epsilon\sin\psi)^k}{k!}\left(\frac{1}{1-\epsilon\cos\psi}\partial_\psi\right)^k\psi \qquad [71]$$

---

① 此标记有问题，原文如此　　译者注。

的求和(Levi-Civita)所表明。

甚至有可能把级数项重新表达为具有更好收敛性质的级数。比如,级数项可以重新组织相加使得 h 表述成以

$$\eta = \frac{\varepsilon e^{\sqrt{1-\varepsilon^2}}}{1+\sqrt{1-\varepsilon^2}} \qquad [72]$$

为参数的幂级数,其收敛半径为 1,对应于 $\varepsilon=1$(利用 Levi-Civita 提供的简单证明)。拉格朗日级数的解析域为 $|\eta|<1$。这也决定了拉普拉斯半径,即复曲线 $|\eta(\varepsilon)|=1$ 到原点最近的距离,它是虚的,为方程

$$\varepsilon e^{\sqrt{1+\varepsilon^2}}/(1+\sqrt{1+\varepsilon^2}) = 1$$

的根。

上述分析提供一个实用方面非常重要的简单例子,通过用作用量-角变量表达扰动函数作出实际上所需的计算。式[66]中函数 $c(\lambda)$ 是余弦函数的性质只是用来把 v 值的范围限制在 ±1 以内,因此,同样的方法当然得到类似的结果,可以用来研究平均偏近点角 λ 和真偏近点角 θ 之间关系的求逆,以及有效地得到如式[42]中的函数 f,g 的性质。

欲知更多的细节,读者可参阅 Levi-Civita(1956)。

Lindstedt 级数与 Birkhoff 级数:发散性

运动常数的非存在性,与其说是用微扰法研究可积系统附近的运动之尝试的终点,勿宁说是理解它们的本质之新努力的起点。

令 $(\boldsymbol{A},\boldsymbol{\alpha})\in U\times\mathbb{T}^l$ 是定义在解析哈密顿量可积性区域上的作用量-角变量,令 $h(\boldsymbol{A})$ 是哈密顿量在作用量-角坐标系中的值。假设 $h(\boldsymbol{A}_0)$ 是非等时性的,$f(\boldsymbol{A},\boldsymbol{\alpha})$ 是一个解析扰动函数。考虑哈密顿量 $\mathcal{H}_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha})=\mathcal{H}_0(\boldsymbol{A})+\varepsilon f(\boldsymbol{A},\boldsymbol{\alpha})$,$\varepsilon$ 为小值。

令 $\boldsymbol{\omega}_0=\boldsymbol{\omega}(\boldsymbol{A}_0)\equiv\partial_A \boldsymbol{H}_0(\boldsymbol{A})$ 为对应作用量 $\boldsymbol{A}_0$ 的未扰动系统的不变圆环面之一的频谱(参见"准周期性与可积性"一节)。已知没有可积性,现在的问题是扰动系统是否有解析的不变圆环面,其上的运动是准周期的,且它

(1)有同样的频谱 $\boldsymbol{\omega}_0$;

(2)至少对小的 ε,它解析地依赖于 ε;

(3)当 $\varepsilon\to0$ 时,它退化为"未扰动圆环面" $\{\boldsymbol{A}_0\}\times\mathbb{T}^l$。

问题可以具体表述如下:

是否存在函数 $\boldsymbol{H}_\varepsilon(\boldsymbol{\psi})$,$\boldsymbol{h}_\varepsilon(\boldsymbol{\psi})$,对于 $\psi\in\mathbb{T}^l$ 和在 0 附近的 ε 是解析的,且当 $\varepsilon\to0$ 为零,使得参数方程为

$$\boldsymbol{A}=\boldsymbol{A}_0+\boldsymbol{H}_\varepsilon(\boldsymbol{\psi}),\qquad \boldsymbol{\alpha}=\boldsymbol{\psi}+h_\varepsilon(\boldsymbol{\psi}),\qquad \boldsymbol{\psi}\in\mathbb{T}^l \qquad [73]$$

的圆环面是不变的?且如果 $\boldsymbol{\omega}_0\overset{\text{def}}{=}\boldsymbol{\omega}(\boldsymbol{A}_0)$,其上的运动简单地为 $\boldsymbol{\psi}\to\boldsymbol{\psi}+\boldsymbol{\omega}_0 t$,即是准周期的?

在此语境下,由庞加莱定理(见"通有不可积性"一节)得到了另一个重要结果(先是对一特例发展起来的,后由庞加莱加以完备的),可以对上述问题给出部分的解答。

假设 $\boldsymbol{\omega}_0=\boldsymbol{\omega}(\boldsymbol{A}_0)\in\mathbb{R}^l$ 满足丢番图性质,即假设存在常数 $C,\tau>0$,使得

$$|\boldsymbol{\omega}_0\cdot\boldsymbol{v}|\geqslant\frac{1}{C|\boldsymbol{v}|^\tau},\text{对所有 } 0\neq\boldsymbol{v}\in\mathbb{Z}^l \qquad [74]$$

对每一个固定的 $\tau>l-1$,这是一个为所有的、但除去零测度集合的 $\boldsymbol{\omega}\in\mathbb{R}^l$ 都满足的性质。由于式[74]暗含的 ω_0 的"无理性",未扰动圆环面上的轨道稠密地充满圆环面。把哈密顿方程写成

$$\dot{\boldsymbol{\alpha}}=\partial_A\mathcal{H}_0(\boldsymbol{A})+\varepsilon\partial_A f(\boldsymbol{A},\boldsymbol{\alpha}),\qquad \dot{\boldsymbol{A}}=-\varepsilon\partial_\alpha f(\boldsymbol{A},\boldsymbol{\alpha})$$

其中的 $\boldsymbol{A},\boldsymbol{\alpha}$ 由式[73]用 $\boldsymbol{\Psi}+\boldsymbol{\omega}t$ 替代 $\boldsymbol{\Psi}$ 而给出;利用式[74]暗指的未扰动轨道的稠密性,则式[73]是其上运动为 $\boldsymbol{\Psi}\to\boldsymbol{\Psi}+\boldsymbol{\omega}_0 t$ 的不变圆环面方程的条件是

$$\begin{aligned}\boldsymbol{\omega}_0+(\boldsymbol{\omega}_0\cdot\partial_\psi)\boldsymbol{h}_\varepsilon(\boldsymbol{\Psi})&=\partial_A\mathcal{H}_0(\boldsymbol{A}_0+\boldsymbol{H}_\varepsilon(\boldsymbol{\Psi}))+\varepsilon\partial_A f(\boldsymbol{A}_0+\boldsymbol{H}_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{\Psi}+\boldsymbol{h}_\varepsilon(\boldsymbol{\Psi}))(\boldsymbol{\omega}_0\cdot\partial_\psi)\boldsymbol{H}_\varepsilon(\boldsymbol{\Psi})\\&=-\varepsilon\partial_\alpha f(\boldsymbol{A}_0+\boldsymbol{H}_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{\Psi}+\boldsymbol{h}_\varepsilon(\boldsymbol{\Psi}))\end{aligned}\qquad[75]$$

同上述问题相联系的定理(Poincaré)为

定理 2 如果未扰动系统是非等时的,且对某些 $C,\tau>0$,$\boldsymbol{\omega}_0=\boldsymbol{\omega}(\boldsymbol{A}_0)$ 满足式[74],则存在两个定义良好的幂级数 $\boldsymbol{h}_\varepsilon(\boldsymbol{\psi})=\sum_{k=1}^{\infty}\varepsilon^k\boldsymbol{h}^{(k)}(\boldsymbol{\psi})$ 和 $\boldsymbol{H}_\varepsilon(\boldsymbol{\psi})=\sum_{k=1}^{\infty}\varepsilon^k\boldsymbol{H}^{(k)}(\boldsymbol{\psi})$,它对 ε 的所有阶都解式[75]。$\boldsymbol{H}_\varepsilon$ 的级数是惟一决定了的,而 $\boldsymbol{h}_\varepsilon$ 的级数在每一阶除去一个未定常数也是如此;因此不失一般性,如果要求 $\boldsymbol{h}_\varepsilon$ 对 $\boldsymbol{\psi}$ 的平均为零,则 $\boldsymbol{h}_\varepsilon$ 也是惟一确定的。

针对一个简单例子的构造算法将在下节介绍(见方程[83]和[84])。上述级数称为 **Lindstedt 级数**,它的收敛性,即使是对小的 ε,长期以来也是个问题。庞加莱证明了形式解的存在;但他的其他结果(已在"通有不可积性"一节讨论过),正如一些作者(包括庞加莱自己)很快就强调的那样,虽然未排除收敛性,但却提出了质疑。那节的结果表明,在给定的谱附近,对所有的 ω_0 解析地一致地解方程[75]是不可能的,但不排除对单一的 ω_0 解此方程的可能性。

此定理有多种扩展或类比。一个有趣的针对未扰动的等时系统的定理是:

给定哈密顿量 $\mathcal{H}_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha})=\boldsymbol{\omega}_0\cdot\boldsymbol{A}+\varepsilon f(\boldsymbol{A},\boldsymbol{\alpha})$,$\omega_0$ 满足[74]而 f 是解析的,则存在幂级数 $C_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}')$ 和 $u_\varepsilon(\boldsymbol{A}')$,使得 $\mathcal{H}_\varepsilon(C_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}'))=\boldsymbol{\omega}_0\cdot\boldsymbol{A}'+u_\varepsilon(\boldsymbol{A}')$ 作为形式幂级数的相等(即关于 ε 逐阶成立),同时 $\boldsymbol{C}_\varepsilon$(看成一个映射)逐阶满足是正则映射的条件①。

这里是指存在一个用形式幂级数,$\boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha})=\sum_{k=1}^{\infty}\varepsilon^k\boldsymbol{\Phi}^{(k)}(\boldsymbol{A}',\boldsymbol{\alpha})$,来定义的生成函数 $\boldsymbol{A}'\cdot\boldsymbol{\alpha}+\boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha})$,即若 $C_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}')=(\boldsymbol{A},\boldsymbol{\alpha})$ 成立,则 $\boldsymbol{A}=\boldsymbol{A}'+\partial_\alpha\boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha})$,$\boldsymbol{\alpha}=\boldsymbol{\alpha}'+\partial_A\boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha})$ 关于 ε 的幂逐阶成立。级数 $\boldsymbol{\Phi}_\varepsilon,u_\varepsilon$ 称为 **Birkhoff 级数**。

在等时系统情形下,如果对小的 ε 和 $(\boldsymbol{A}',\boldsymbol{\alpha})$ 在形式为 $U\times\mathbb{T}^l$,$U\subset\mathbb{R}^l$ 是开的、有限的某区域内 Birkhoff 级数是收敛的,则 $\mathcal{H}_\varepsilon$ 对小的 ε 会在相空间较大的区域内(即在生成函数可以用来构造正则映射的地方,实际上是 $U\times\mathbb{T}^l$ 去掉 U 的边界附近一小层点)是可积的。可是,对小的 ε 的收敛性(一般地)是不成立的,这可由下面的简单二维例子来说明:

$$\left.\begin{aligned}&\mathcal{H}_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha})=\boldsymbol{\omega}_0\cdot\boldsymbol{A}+\varepsilon(\boldsymbol{A}_2+f(\boldsymbol{\alpha}))\\&(\boldsymbol{A},\boldsymbol{\alpha})\in\mathbb{R}^2\times\mathbb{T}^2\end{aligned}\right\}\qquad[76]$$

其中 $f(\boldsymbol{\alpha})$ 是其傅里叶系数 $f_0=0$,$\boldsymbol{v}\neq0$ 而所有其他系数 f_v 都为正的任意解析函数。在这个例子中,解为

① 即(4.3)。不知何指——原文如此,译者注。

$$\left.\begin{aligned} u_\varepsilon(\boldsymbol{A}') &= \varepsilon A_2 \\ \boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}) &= \sum_{k=1}^{\infty}\varepsilon^k \sum_{0\neq v\in Z^2} f_v \mathrm{e}^{\mathrm{i}\boldsymbol{\alpha}\cdot v}\frac{(\mathrm{i}v_2)^k}{(\mathrm{i}(\omega_{01}v_1+\omega_{02}v_2))^{k+1}} \end{aligned}\right\} \quad [77]$$

上述级数不收敛。实际上它的收敛性意味着可积性,因此就意味着相空间中轨道的有界性。但是运动方程[76]的显式的解很容易给出,而且如果 $\omega_{01}/(\omega_{02}+\varepsilon)$ 是有理的,则在任何给定的初始条件附近的任何开域内总有无界的轨道。

但是,即使在这样基本的情形下,对级数的形式求和可得

$$\left.\begin{aligned} u(\boldsymbol{A}') &= \varepsilon A_2' \\ \boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}) &= \varepsilon \sum_{0\neq v\in Z^2}\frac{f_v \mathrm{e}^{\mathrm{i}\boldsymbol{\alpha}\cdot v}}{\mathrm{i}(\omega_{01}v_1+(\omega_{20}+\varepsilon)v_2)} \end{aligned}\right\} \quad [78]$$

而如果 $\boldsymbol{\omega}=(\omega_{01},\omega_{02}+\varepsilon)$ 是丢番图矢量(根据式[74],解析性意味着 $|f_v|$ 指数衰减),则式[78]中的级数(不再是 ε 的幂级数)确实是收敛的。值得注意的是,尽管式[78]是由式[77]通过不严格的求和规则

$$\sum_{k=0}^{\infty} z^k = \frac{1}{1-z}, z\neq 1 \quad [79]$$

(应用到 $|z|\geqslant 1$ 的情形。因为 $z=v_2/\boldsymbol{\omega}_0\cdot\boldsymbol{v}$,如果 $\boldsymbol{\omega}$ 是丢番图的,这样的情形当然能对 ε 的一个稠集实现)得到的,对那样的 ε 值,哈密顿量 $\mathcal{H}_\varepsilon$ 可以由式[78]生成的正则映射进行积分,因而是可积的。换句话说,方程的可积性是基本的,只要 $\boldsymbol{\omega}$ 是丢番图的,则解可以从式[78]严格得到。这意味着,举例来说,像 $\sum_{k-0}^{\infty} 2^k = -1$ ①这样的关系确实可以用来从式[77]得到式[78]。

Lindestedt 级数的另一个推广出现在处理非等时系统的扰动时,问未扰动的、其上谱是共振(即对某些 $\boldsymbol{v}\neq 0, \boldsymbol{v}\in\mathbb{Z}^l$,有 $\boldsymbol{\omega}_0\cdot\boldsymbol{v}=0$)的不变圆环面 $\mathcal{T}_{\omega_0}$ 上会发生什么。其结果是,即使在这种情形下,存在一个形式幂级数的解,在 $\varepsilon\neq 0$ 时可以形式上加以延拓,这个形式解表明至少有一些(无穷多)不变圆环面,在未扰动的情况下 $\mathcal{T}_{\omega_0}$ 可以分叶成这些圆环面的叶状结构(参见"共振及其稳定性"一节)。

欲知更多的细节,读者可参阅 Poincaré (1987)。

准周期性与 KAM 稳定性

为了讨论更深入的结果,我们把注意力局限在特殊的(非平凡的)范例

$$H_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha}) = \frac{1}{2}\boldsymbol{A}^2 + \varepsilon f(\boldsymbol{\alpha}) \quad [80]$$

上。在这样的简单情形下(称为 **Thirring 模型**,描述 l 个粒子在圆上通过势 $\varepsilon f(\alpha)$ 相互作用),最大圆环面的方程[75]约化成只是函数 $\boldsymbol{h}_\varepsilon$ 的方程

$$(\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\Psi}})^2\boldsymbol{h}_\varepsilon(\boldsymbol{\Psi}) = -\varepsilon\partial_\alpha f(\boldsymbol{\Psi}+\boldsymbol{h}_\varepsilon(\boldsymbol{\Psi})),\ \boldsymbol{\Psi}\in\mathbb{T}^l \quad [81]$$

因为式[75]的第二式右边不含 $\boldsymbol{H}_\varepsilon$,故变成了对 $\boldsymbol{H}_\varepsilon$ 的定义。

实际的问题因此就变成了上一节考虑的形式级数是否对小的 ε 是收敛的,关于 Birk-

① 原文如此,指将 $z=2$ 代入式[79]——译者注。

hoff 级数的例子式[76]表明有时候需要求和规则以便为级数赋予含义。实际上,只要(有物理意义的)问题有不收敛的,或收敛性不确定的形式幂级数解,就应该找寻求和规则。

微扰论的近代理论开始于 Lindestedt 级数对小的 ε 收敛性的证明(Kolmogorov)。一般的"KΛM"结果是:

定理 3(KΛM) 考虑哈密顿量 $\mathcal{H}_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha})=h(\boldsymbol{A})+\varepsilon f(\boldsymbol{A},\boldsymbol{\alpha})$,其定义在 $U\times\mathbb{T}^r(U\subset\mathbb{R}^r$ 是开的、有限的)某区域上,且 $f(\boldsymbol{A},\boldsymbol{\alpha})$ 和 $h(\boldsymbol{A})$ 在闭包 $\bar{V}\times\mathbb{T}^r$ 上是解析的,$h(A)$ 还是非等时的;令 $\boldsymbol{\omega}_0\overset{\text{def}}{=}\boldsymbol{\omega}(\boldsymbol{A}_0)=\partial_A h(\boldsymbol{A}_0)$ 且假设 $\boldsymbol{\omega}_0$ 满足式[74],则

(i)存在 $\varepsilon_{C,\tau}>0$,Lindestedt 级数对于 $|\varepsilon|\leqslant\varepsilon_{C,\tau}$ 是收敛的;

(ii)其求和得到 $\mathbb{T}^r$ 上的两个函数 $\boldsymbol{H}_\varepsilon(\boldsymbol{\psi})$,$\boldsymbol{h}_\varepsilon(\boldsymbol{\psi})$,这两个函数参数化一个不变圆环面 $\mathcal{T}_{C,\tau}(\boldsymbol{A}_0,\varepsilon)$;

(iii)$\mathcal{T}_{C,\tau}(\boldsymbol{A}_0,\varepsilon)$ 上的运动为 $\boldsymbol{\psi}\to\boldsymbol{\psi}+\omega_0 t$,参见式[73];

(iv)对预先给定的 C,τ,以及 $\boldsymbol{\omega}(\boldsymbol{A}_0)$ 满足[74],在不变圆环面 $\mathcal{T}_{C,\tau}(\boldsymbol{A}_0,\boldsymbol{\varepsilon})$ 中存在一个初始条件集合 U,它的补集合其体积<常数$\times C^{-a}$($a>0$ 为适当常数),其在每一个常能量面,$\mathcal{H}_\varepsilon=E$ 上也有面积<常数$\times C^{-a}$。

换句话说,对小的 ε,大部分未扰动的准周期运动的谱可以发现是扰动的在圆环面(接近未扰动的)上的准周期运动的谱(即有同样的谱)。

这是一个稳定性结果:举例来说,对一个两自由度的系统,其在三维能量面上的二维不变圆环面会把能量面上的点分成圆环面"内"和"外"两个集合。因此,初始数据在"内"部开始不会到达"外"部。类似的,在两个圆环面中间开始的点会永远停留在两者之间。进一步,如果两个圆环面是闭合的,这意味着运动在作用量空间是局域的,其轨道只能划过那些接近圆环面的点且接近所有的这样的点:离那些点的距离同被约束其上的圆环面间的距离可比拟。三维或更多维的情况完全不同(参见"相空间的扩散"和"三体问题"两节内容)。

在像式[80]转子系统那样的简单情形下,圆环面的参数化表示的方程由式[81]给出。这个问题同式[66]中较容易的问题有些类似:但式[81]中有 r 个方程而不是一个方程,它们是微分方程而不是普通方程。而且,扮演式[66]中 $c(\lambda)$ 角色的函数 $f(\boldsymbol{\alpha})$,其傅里叶系数 f_v 对 $\boldsymbol{v}$ 没有限制,而式[66]中 c 的傅里叶系数 c_v 只当 $v=\pm1$ 时才不为零。

上述的区别某种程度上是"微小的"且式[81]的幂级数解可以用对式[66]用过的相同算法构造,即可以形成图 5 中那样的树,但用 $\boldsymbol{v}_v\in\mathbb{Z}^r$(仍然可以认为是扰动函数 f 的傅里叶展开中的谐波指标)取代谐波标签 $v_v\in\mathbb{Z}$。其他的在"定属不可积性"一节中贴在树上的标签不变。特别是,沿分枝 $l=v'v$ 的流定义为在节点 v 之前所有节点 $w\leqslant v$ 的谐波的和

$$\boldsymbol{v}(l)\overset{\text{def}}{=}\sum_{w\leqslant v}\boldsymbol{v}_w \qquad [82]$$

我们称 $\boldsymbol{v}(\theta)$ 为流过根部的流。

这里树的值 $\mathrm{Val}(\theta)$ 必须以不同方式定义,因为这里要解的方程([81])含有微分算符 $(\boldsymbol{\omega}_0\cdot\partial_{\boldsymbol{\psi}})^2$,其傅里叶变换的系数为谐波 $\boldsymbol{v}$ 的傅里叶分量乘积,为 $(\mathrm{i}\boldsymbol{\omega}_0\cdot\boldsymbol{v})^2$。

由算符 $(\mathrm{i}\omega_0\cdot v)^2$ 的出现以及在计算 $\boldsymbol{u}\cdot\boldsymbol{h}_v^{(k)}$(即 $\boldsymbol{h}_v^{(k)}$ 沿任意单位矢量 $\boldsymbol{u}$ 方向上的分量)必须对其作反变换所带来的变化却是非常简单的:一个 k 阶(k 个节点,k 个分枝)树图

θ 的值须由

$$\mathrm{Val}(\theta)\overset{\mathrm{def}}{=}\frac{-\mathrm{i}(-1)^k}{k!}\Big(\prod_{\mathrm{lines}\,l=v'v}\frac{\boldsymbol{v}_{v'}\cdot\boldsymbol{v}_v}{(\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l))^2}\Big)\times\Big(\prod_{\mathrm{nodes}}\boldsymbol{f}_{v_v}\Big)\qquad[83]$$

来定义(比较式[68]),这里出现在联系着从第一节点 v 到根 r 的根线 rv (见图 5)因子里的 $v_{v'}$ 可理解为一个单位矢量 $\boldsymbol{u}$(在[66]一维情形下它被理解为数 1)。方程[83]只对没有携带零流的连线的树才是有意义的,则 $\boldsymbol{h}^{(k)}$ 沿 $\boldsymbol{u}$(联系树根的谐波标签)的分量由式(见式[69])

$$\boldsymbol{u}\cdot\boldsymbol{h}_v^{(k)}=\sum_{\substack{\theta,v(\theta)=v\\ \mathrm{order}(\theta)=k}}^{*}\mathrm{Val}(\theta)\qquad[84]$$

给出,这里 * 的意思是求和只对其中沿连线 $l\in\theta$ 流动的流 $\boldsymbol{v}(l)$ 非零的树进行。量 $\boldsymbol{u}\cdot\boldsymbol{h}_0^{(k)}$ 定义为 0(见前一节)。

在式[66]的情形中可能出现零流的连线,但来自包含至少一根零流连线的树图的贡献抵消了。对于当前的情况,断言通过简单地忽略包含零流连线的树图,上述算法仍给出 $\boldsymbol{h}^{(k)}$ 并非无关重要的。来自庞加莱的对 Lindestedt 级数理论的贡献表明,即使是在一般情况下(比较式[75]),不变圆环面的方程也能用形式幂级数求解。通过验证前几项,方程[84]由归纳法可证。

前述导出式[83]的算法可以推广到 KAM 定理考虑的一般性的哈密顿量上。

收敛性证明比方程[66]的初级证明要微妙一些。实际上,k 阶树图对 $\boldsymbol{h}_v^{(k)}$ 的贡献较大,因为新因子 $(\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l))^2$,尽管不为零,但其小的程度要超过因子 f_v 和 ε。实际上,即使 f 是一个三角多项式(f_v 对足够大的 $|\boldsymbol{v}|$ 一致为零),分支里流动的流可以非常大,同树的节点数 k 同量级,见式[82]。

这就是所谓的**小除数问题**,解决该问题的关键可回溯到相关工作(Siegel),有:

定理 4 *考虑树图 θ 对式[82]中求和的贡献,树图中没有一对在到根部的相同路径上的连线携带同样的流,且节点谐波是有界的,即对某些 N,$|\boldsymbol{v}|\leqslant N$,树图 θ 中其除数 $\boldsymbol{\omega}_0\cdot\boldsymbol{v}_l$ 满足 $2^{-n}<C|\boldsymbol{\omega}_0\cdot\boldsymbol{v}_l|\leqslant 2^{n+1}$ 的连线的个数 l 不超过 $4Nk2^{-n/\tau}$。*

因此,令

$$F\overset{\mathrm{def}}{=}C^2\max_{|\boldsymbol{v}|\leqslant N}|f_{\boldsymbol{v}}|$$

则相应的值 $\mathrm{Val}(\theta)$ 的上限为

$$\left.\begin{aligned}&\frac{1}{k!}F^kN^{2k}\prod_{n=0}^{(*)}2^{2n(4Nk2^{-n/\tau})}\overset{\mathrm{def}}{=}\frac{1}{k!}B^k\\ &B=FN^2 2\sum_n 8n2^{-n/\tau}\end{aligned}\right\}\qquad[85]$$

因为乘积是收敛的。当 f 是 N 次的三角多项式时,上述对 $\boldsymbol{u}\cdot\boldsymbol{h}_v^{(k)}$ 的受限的贡献会产生一个对足够小的 ε 收敛的级数。实际上,树的数目是有界的(见"扰动函数"一节),为 $k!\,4^k(2N+1)^{lk}$,则级数 $\sum_v|\varepsilon|^k|\boldsymbol{u}\cdot\boldsymbol{h}_v^{(k)}|$ 对小的 ε(即 $|\varepsilon|<(B\cdot 4(2N+1)^l)^{-1}$)收敛。

据此,对"剩余贡献"的分析真正成问题了,需要新的思路才行,因为在排除掉的树图中有某些简单的第 k 阶树,如果从其他贡献分别考虑,单是它们的值就会产生一个阶乘发散的关于 ε 的幂级数。

但是,所有大数值的 k 阶树的贡献是抵消的。尽管不是严格抵消的(不像在"扰动函数"一节里讨论的初等情形,那里的证明不需用到抵消的性质,虽然抵消确实发生了),但程度足够保证尽管某些单个的树图的值特别大,树图值的和的上界不超过某常数的 k 次幂,从而级数对足够小的 ε 收敛。相关讨论见附录一。

欲知更多的细节,读者可参阅 Poincaré(1987),Kolmogorov(1954),Moser(1962)和 Arnol′d(1989)。

共振及其稳定性

具有 r 个独立的有理频率的准周期运动,如果 r 严格少于自由度数 l,则称为是共振的,两者之差 $l-r$ 为共振度。

特别有意义的是对可积系统的扰动,那里就发生共振运动。

一个典型的例子是研究围绕一个大质量粒子的 $n-1$ 个粒子间受引力作用相互扰动的 n 体问题。如果粒子质量[①]可以忽略不计,系统则是由 $n-1$ 个开普勒有心运动构成,其自由度为 $l=3(n-1)$。一般地,若无相互扰动,每个运动只有一个频率(即开普勒轨道的周期)。因此,$r\leqslant n-1$,$s\geqslant 2(n-1)$(在平面内的运动,$s\geqslant(n-1)$),当周期为相互之间有理独立的则等式成立。

另一个例子是受到保守力扰动的绕固定点的刚体运动,未扰动的系统有 3 个自由度,但一般地只有两个频率(见基于式[52]的讨论)。

进一步,上述例子中存在这样的可能:在某些特殊的初始条件下,独立的频率的值是有理相关的,因此会有更高阶的共振(即更小的 r 值)。

在可积非等时系统中,共振运动在相空间里是稠密的,因为频率 $\boldsymbol{\omega}(\boldsymbol{A})$ 会像作用量一样变化,所以任何阶(对任何 $r<l$)的共振在相空间里都是稠密的;特别地,周期运动(即最高阶共振)是稠密的。

可积系统的共振可以出现在先验稳定的可积系统和先验不稳定系统中,前者是哈密顿量允许正则作用量-角坐标$(\boldsymbol{A},\boldsymbol{\alpha})\in U\times\mathbb{T}^l$($U\in\mathbb{R}^l$ 是开的)系统,而后者在合适的局域正则坐标系中,其哈密顿量的形式为

$$\left.\begin{aligned} &H_0(\boldsymbol{A})+\sum_{i=1}^{s_1}\frac{1}{2}(p_i^2-\lambda_i^2q_i^2)+\sum_{j=1}^{s_2}\frac{1}{2}(\pi_j^2+\mu_j^2\kappa_j^2)\\ &\lambda_i,\mu_j>0 \end{aligned}\right\} \qquad [86]$$

其中$(\Lambda,\alpha)\in U\times\mathbb{T}^r$,$U\in\mathbb{R}^r$,$(\boldsymbol{p},\boldsymbol{q})\in V\subset\mathbb{R}^{2s_1}$,$(\boldsymbol{\pi},\boldsymbol{\kappa})\in V'\subset\mathbb{R}^{2s_2}$,$V$,$V'$ 是原点的邻域,而 $l=r+s_1+s_2$,$s_i\geqslant 0$,$s_1+s_2>0$,$\pm\sqrt{\lambda_j}$,以及 $\pm\sqrt{\mu_j}$ 是共振的李雅普诺夫指数。所考虑的扰动形似为 $\varepsilon f(\boldsymbol{A},\boldsymbol{\alpha},\boldsymbol{p},\boldsymbol{q},\boldsymbol{\pi},\boldsymbol{\kappa})$。所谓先验稳定或不稳定的说法指的是原先给定的未扰动的哈密顿量的性质。若 $s_1>0$,"先验不稳定"的标签是合适的,这里允许 $s_1=0$,只是为了记号的方便,意味着先验不稳定的系统情形的李雅普诺夫指数都是 1 量级的(不管是实的 λ_j 还是虚的 $\mathrm{i}\sqrt{\mu_j}$)。换句话说,先验稳定的情形,式[86]中 $s_1=s_2=0$ 是惟一的例外。当然,这两种情况下加上扰动后运动的稳定性质取决于扰动。

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① 应是 $n-1$ 个小质量粒子的质量 译者注。

先验稳定的系统通常有大量的共振(比如,在非等时系统,任何维的共振都是稠密的)。而先验不稳定的系统(在其可能的共振中)有一些特殊的 r 维的共振发生在不稳定坐标($\boldsymbol{p},\boldsymbol{q}$)和($\boldsymbol{\pi},\boldsymbol{\kappa}$)为零时,其 r 个作用量-角坐标的频率是有理独立的。

第一种情况下(先验稳定)的一般性的问题是,充满 l 维不变圆环面排列成簇的 r 维不变圆环面所形成的共振运动,当加上足够小的扰动 $\varepsilon f(A,\alpha)$ 后,在稍微形变的不变圆环面上能否继续存在?对先验不稳定的系统可以提出类似的问题。为了深入考察这个问题,先考虑最简单问题的表述。

先验稳定共振:确切的,假设 $\mathcal{H}_0=\frac{1}{2}\boldsymbol{A}^2$,令$\{\boldsymbol{A}_0\}\times\mathbb{T}^r$为未扰动的不变圆环面$\mathbb{T}_{A_0}$,其谱为 $\boldsymbol{\omega}_0=\boldsymbol{\omega}(\boldsymbol{A}_0)=\partial_{A_0}(\mathcal{H}(A_0))$,只有 r 个有理独立分量。为简单起见,假设 $\boldsymbol{\omega}_0=(\boldsymbol{\omega}_1,\cdots,\boldsymbol{\omega}_r,0,\cdots,0)\overset{\text{def}}{=}\omega\in\mathbb{R}^r$。更一般的,$\omega$ 有 r 个有理独立分量的情况可以通过正则线性坐标变换约化成上述的特例,代价是 $\mathcal{H}_0$ 变成一个虽然仍是作用量的二次型,但是含有乘积项 A_iB_j 的新哈密顿量。但是这样的一般形式的 $\mathcal{H}$ 不会影响当前问题的讨论。

区分"快"角变量 $\alpha_1,\cdots,\alpha_r$ 和"共振"(也称"慢"或"久期"的)角变量 $\alpha_{r+1},\cdots,\alpha_l$,且记 $\boldsymbol{\alpha}=(\boldsymbol{\alpha}',\boldsymbol{\beta})$,$\alpha'\in\mathbb{T}^r$,$\beta\in\mathbb{T}^s$,能带来某些方便。类似地,可以区分"快"作用量 $A_1,\cdots,A_r$ 和"共振"作用量 $B_{r+1},\cdots,B_l$,且记 $A=(A',B)$,$A'\in\mathbb{R}^r$,$B\in\mathbb{R}^s$。

因此,圆环面$\mathbb{T}_{A_0}$,$\boldsymbol{A}_0=(\boldsymbol{A}_0{}',\boldsymbol{B}_0)$是不变圆环面 $\mathcal{T}_{A_0,\beta}$的连续体,其参数方程是平凡的:$\boldsymbol{\beta}$ 固定,$\boldsymbol{\alpha}'=\boldsymbol{\psi}$,$\boldsymbol{\psi}\in\mathbb{T}^r$,且 $\boldsymbol{A}'=\boldsymbol{A}_0{}'$,$\boldsymbol{B}=\boldsymbol{B}_0$。在每个不变圆环面上,运动可表述为:$\boldsymbol{A}'$,$\boldsymbol{B}$,$\boldsymbol{\beta}$ 保持不变,$\boldsymbol{\alpha}'\to\boldsymbol{\alpha}'+\boldsymbol{\omega}t$,$\omega\in\mathbb{R}^r$ 是有理独立的。

很自然的要问,是否存在函数 $\boldsymbol{h}_\varepsilon,\boldsymbol{k}_\varepsilon,\boldsymbol{H}_\varepsilon,\boldsymbol{K}_\varepsilon$,它们定义在 $\boldsymbol{\Psi}\in T^r$ 上,在 $\varepsilon=0$ 附近是光滑的,当 $\varepsilon=0$ 为零,使得参数方程为

$$\left.\begin{aligned}&\boldsymbol{A}'=\boldsymbol{A}'_0+\boldsymbol{H}_\varepsilon(\boldsymbol{\Psi}),\ \boldsymbol{\alpha}'=\boldsymbol{\Psi}+\boldsymbol{h}_\varepsilon(\boldsymbol{\Psi}),\\&\boldsymbol{B}=\boldsymbol{B}_0+\boldsymbol{K}_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{\beta}=\boldsymbol{\beta}_0+\boldsymbol{k}_\varepsilon(\boldsymbol{\Psi}),\ \boldsymbol{\Psi}\in\mathbb{T}^r\end{aligned}\right\}\tag{87}$$

的圆环面 $T_{\boldsymbol{A}_0,\boldsymbol{\beta}_0,\varepsilon}$对于哈密顿量 $\mathcal{H}_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha})=\frac{1}{2}\boldsymbol{A}'^2+\frac{1}{2}\boldsymbol{B}^2+\varepsilon f(\boldsymbol{\alpha}',\boldsymbol{\beta})$的运动方程是不变的,且在其上的运动方程为 $\boldsymbol{\Psi}\to\boldsymbol{\Psi}+\boldsymbol{\omega}t$?上述性质如果得到满足,可以简述为未扰动的共振运动 $\boldsymbol{A}=(\boldsymbol{A}_0{}',\boldsymbol{B}_0)$,$\boldsymbol{\alpha}=(\boldsymbol{\alpha}_0{}'+\boldsymbol{\omega}'t,\boldsymbol{\beta}_0)$在扰动 εf,ε 为小参数的作用下可以连续地转变成在稍微形变的圆环面 $T_{A'_0,\beta_0,\varepsilon}$上的相同谱函数的准周期运动。

先验不稳定共振:这里的问题是,在足够小的扰动下特殊的不变圆环面是否继续存在?当然若存在应该有稍微形变。这意味着问,给定 $\boldsymbol{A}_0$使得 $\boldsymbol{\omega}(\boldsymbol{A}_0)=\partial_A(\mathcal{H}_0(\boldsymbol{A}_0))$有有理独立的分量,是否存在具有如下性质函数$(\boldsymbol{H}_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{h}_\varepsilon(\boldsymbol{\Psi}))$,$(\boldsymbol{P}_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{Q}_\varepsilon(\boldsymbol{\Psi}))$和$(\boldsymbol{\Pi}_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{K}_\varepsilon(\boldsymbol{\Psi}))$,它们定义在$\boldsymbol{\psi}\in\mathbb{T}^r$上,在 $\varepsilon=0$ 附近是光滑的,当 $\varepsilon=0$ 为零,且使得 r 维表面

$$\left.\begin{aligned}&\boldsymbol{A}=\boldsymbol{A}_0+\boldsymbol{H}_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{\alpha}=\boldsymbol{\Psi}+\boldsymbol{h}_\varepsilon(\boldsymbol{\Psi})\\&\boldsymbol{p}=\boldsymbol{P}_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{q}=\boldsymbol{Q}_\varepsilon(\boldsymbol{\Psi})\qquad\boldsymbol{\Psi}\in\mathbb{T}^r\\&\boldsymbol{\pi}=\boldsymbol{\Pi}_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{\kappa}=\boldsymbol{K}_\varepsilon(\boldsymbol{\Psi})\end{aligned}\right\}\tag{88}$$

是不变圆环面 $\mathcal{T}_{A_0,\varepsilon}$,其上的运动为 $\boldsymbol{\Psi}\to\boldsymbol{\Psi}+\boldsymbol{\omega}(\boldsymbol{A}_0)t$?同样,上述性质可以简述为未扰动的共振运动 $A=(A_0{}',B_0)$,$\alpha=(\alpha_0{}'+\omega't,\beta_0)$在扰动 εf(ε 为小参数)的作用下可以连续地转变成在稍微形变的圆环面 $\mathcal{T}_{A_0,\varepsilon}$上的有相同谱函数的准周期运动。

对上述问题的一些回答将在下节介绍。欲知更多的细节，读者可参阅 Gallavotti et al.(2004)。

共振与 Lindestedt 级数

我们针对哈密顿量 $\mathcal{H}_0(\boldsymbol{A})$ 为 $\frac{1}{2}\boldsymbol{A}^2$（比较式[80]）的范例来讨论方程[87]。因为 $\boldsymbol{\omega}(\boldsymbol{A}')\equiv\boldsymbol{A}'$，所以 $\boldsymbol{A}_0=\boldsymbol{\omega}$，$\boldsymbol{B}_0=0$，扰动 $f(\boldsymbol{\alpha})$ 可以看成是 $\boldsymbol{\alpha}=(\boldsymbol{\alpha}',\boldsymbol{\beta})$ 的函数，令 $\bar{f}(\boldsymbol{\beta})$ 为其对 α' 的平均。

这种情况下，确定上节讨论过的意义下的连续 r 维不变圆环面将是容易理解的。

圆环面 $\mathcal{T}_{\boldsymbol{A}_0,\boldsymbol{B}}$ 中具有参数方程可延拓为形式上 ε 的幂级数的共振不变圆环面是圆环面 $\mathcal{T}_{\boldsymbol{A}_0,\boldsymbol{\beta}_0}$，其中 $\boldsymbol{\beta}_0$ 是平均扰动于 $\bar{f}(\boldsymbol{\beta})$ 的驻点，亦即其平衡点，$\partial_{\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)=0$。事实上，下述定理成立。

定理 5 如果 $\boldsymbol{\omega}\in\mathbb{R}^r$ 满足丢番图性质，且 $\boldsymbol{\beta}_0$ 是"快角的平均" $\bar{f}(\boldsymbol{\beta})$ 的一非退化的驻点（即 $\partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)\neq 0$），则函数 h_ε，k_ε 的下列方程

$$\left.\begin{aligned}(\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\Psi}})^2\boldsymbol{h}_\varepsilon(\boldsymbol{\Psi}) &= -\varepsilon\partial_{\boldsymbol{\alpha}'}f(\boldsymbol{\Psi}+h_\varepsilon(\boldsymbol{\Psi}),\boldsymbol{\beta}_0+k_\varepsilon(\boldsymbol{\Psi}))\\ (\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\Psi}})^2k_\varepsilon(\boldsymbol{\Psi}) &= -\varepsilon\partial_{\boldsymbol{\beta}}f(\boldsymbol{\Psi}+h_\varepsilon(\boldsymbol{\Psi})+k_\varepsilon(\boldsymbol{\psi}))\end{aligned}\right\}\qquad[89]$$

可以有 ε 幂级数的形式解。

因为哈密顿量[80]的简单性，故无需讨论函数 $\boldsymbol{H}_\varepsilon$，$\boldsymbol{K}_\varepsilon$，因为它们所遵从的方程变成了对它们的定义，正如在"准周期性与 KAM 稳定性"一节中的那样，也是因为同样的原因如此。

换句话说，共振圆环面也有 Lindestedt 级数表示，但该级数一般不会是收敛的。

从物理上来说，这一新性质是因为在对圆环面 $\mathcal{T}_{\boldsymbol{A}_0,\boldsymbol{\beta}_0}$ 附近的运动做线性化处理时会引入绕 $\mathcal{T}_{\boldsymbol{A}'_0,\boldsymbol{\beta}_0}$ 的振荡，其频率正比于矩阵 $\varepsilon\partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)$ 的正特征值的平方根；因此，直观上可以预期有必要对矢量 $(\boldsymbol{\omega},\sqrt{\varepsilon\mu_1},\cdots)$（其中 $\varepsilon\mu_j$ 是正的特征值）要求一丢番图性质。由此，那些使得 $(\boldsymbol{\omega},\sqrt{\varepsilon\mu_1},\cdots)$ 不是丢番图矢量，或非常接近丢番图矢量的 ε 应该被排除，或至少预期会造成某些困难。注意，不管是否假设矩阵 $\partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)$ 的非退化性（因为 ε 可正可负），不管假设 $|\varepsilon|$ 有多小，都会出现问题。但我们可以预期，如果矩阵 $\partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)$（比如说）是正定的（即 $\boldsymbol{\beta}_0$ 是 $\bar{f}(\boldsymbol{\beta})$ 的最小点），则问题对 $\varepsilon<0$ 会很容易；或者反过来，若 $\boldsymbol{\beta}_0$ 是 $\bar{f}(\boldsymbol{\beta})$ 的最大点，则问题对 $\varepsilon>0$ 会很容易（即是这样的情况，矩阵 $\partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)$ 的特征值为负，其平方根不能理解为频率）。

从技术上讲，形式级数的和只有通过涉及发散级数的求和才可以赋予某个意义。典型的做法是，找出形式表述中（可数个）几何级数，几何级数虽然是发散的，但却可以通过求和规则[79]获得意义。因为只当 $z\neq 1$ 时才能使用求和规则，这就引出了对参数 ε 的条件以避免不得不考虑 z 非常接近于 1 的情形。所以，这个稳定性就和 KAM 关于最大圆环面的稳定性不一样。可以说，如果 f 和 $\boldsymbol{\beta}_0$ 满足某些附加条件，且某些 ε 的值被排除掉，就能通过求和规则给级数赋予某个意义。举例来说，有如下定理。

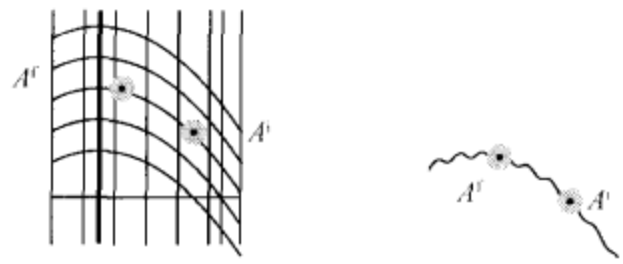
定理 6 给定哈密顿量[80]和一个共振圆环面 $\mathcal{T}_{\boldsymbol{A}'_0,\boldsymbol{\beta}_0}$，其中 $\boldsymbol{\omega}=\boldsymbol{A}'_0\in\mathbb{R}^r$ 满足丢番图

性质,$\boldsymbol{\beta}_0$ 是平均势能 $f(\boldsymbol{\beta}) \overset{\text{def}}{=} (2\pi)^{-r}\int_{T^r} f(\boldsymbol{\alpha}', \boldsymbol{\beta})\mathrm{d}^r\boldsymbol{\alpha}'$ 的非退化的最大值点。考虑谱为 $(\boldsymbol{\omega}, 0)$ 的扰动共振圆环面的方程[89]的 Lindestedt 级数形式解。可以把级数的单一 n-阶项表达为许多项的和,然后重新安排所得到的级数,使新级数对在域 $\mathcal{E}$ 中的 ε 收敛;域 $\mathcal{E}$ 含片段 $[0, \varepsilon_0]$ 和 $[-\varepsilon_0, 0]$ 的子集(尽管有开而稠的补集,但它足够大,可以有 0 作为它的勒贝格密度点)。进一步,关于 $\boldsymbol{h}_\varepsilon, \boldsymbol{k}_\varepsilon$ 的新级数定义了一个谱为 $\boldsymbol{\omega}$ 的 r 维不变的解析圆环面。

更一般地,如果 $\boldsymbol{\beta}_0$ 只是 $\bar{f}(\beta)$ 的非退化的驻点,重新安排级数的定义域是集合 $\mathcal{E} \subset [-\varepsilon_0, \varepsilon_0]$,它尽管有 0 作为它的勒贝格密度点,但在原点两侧都有开而稠的补集。

如果 $\partial^2_{\boldsymbol{AA}} h$ 是非奇性的矩阵,且共振来自有 r 个独立分量(其他分量不需要为零)的谱 $\boldsymbol{\omega}(\boldsymbol{A}_0)$,则定理 6 可以自然地推广到一般情况,哈密顿量是对非等时可积系统 $H_\varepsilon(\Lambda, \alpha) = h(A) + \varepsilon f(\boldsymbol{A}, \boldsymbol{\alpha})$ 的最一般的扰动。

对近似可积共振运动的 Lindstedt 级数,收敛性是一个微妙的问题。级数甚至可能是发散的(发散性的数学证明还是个悬而未决的问题,而从前述物理诠释的观点来看却是相当合理的推测);但是,定理 6 表明有时(比如,ε 在 $\varepsilon = 0$ 附近足够大的集合内)求和规则能够给出问题的真解。



(a)　(b)

图 6　(a)$\varepsilon = 0$ 的几何。"部分能量"线是抛物线,$(1/2)A_1^2 + A_2 =$ 常数。竖直线是共振 $A_1 =$ 有理数(即 $\boldsymbol{v}_1 A_1 + \boldsymbol{v}_2 = 0$)。圆盘是点 A^i 和 A^f(圆盘的中心)的邻域。(b)$\varepsilon \neq 0$:空间 Λ 中一条轨道的艺术家画法。轨道被单摆的摆动所驱动,以时钟的能量为代价把轮子从 A^i 加速到 A^f。它穿过不变圆环面(未画出),且(近似地)远离共振和部分能量线(一个稠集)的交点。单摆的坐标未画出,但它的能量在 ε 量级上停留在 0 附近。因此单摆的摆动停留在分隔曲线的附近。震荡表示的是部分能量 $(1/2)A_1^2 + A_2$ 在不变(没有单摆的存在是不可能的)圆环面之间潜行的过程中的摇摆行为。轮子的能量 $(1/2)A_1^2$ 在单摆每次摆动后增加一点,精确的估计得出轮子速度在单摆每次摆动后的增加为 $\varepsilon/(\lg\varepsilon^{-1})$ 量级,对应的过渡时间为 $g^{-1/2}\varepsilon^{-1}\lg\varepsilon^{-1}$ 量级。

这让人想起了讨论式[76]中的等时系统扰动所遇到的现象,但形势却更加复杂。有许多悬而未决的问题:最关键的是惟一性问题。发散级数的求和规则总含有一些随意的选择,因此会留下对由此构造的参数化不变圆环面的函数之惟一性的疑问。甚至收敛集 $\mathcal{E}$ 依赖于那些随意的选择,考虑几个选择后会发现没有 $|\varepsilon| < \varepsilon_0$ 的 ε 被省略去。

先验不稳定系统的情形也已被充分研究,也考虑了具有丢番图性质的谱为 r 维 ω 的共振。但是,在 $s_2 = 0$ 的情况下(称为先验不稳定双曲共振),可证 Lindestedt 级数是收敛的,而在 $s_1 = 0$(称为先验不稳定椭圆共振)或在混合的 $s_1, s_2 > 0$ 情况下,则需要附加条件,需要涉及 $\boldsymbol{\omega}$ 和 $\boldsymbol{\mu} = (\mu_1, \cdots, \mu_{s2})$(参见式[86])以及扰动本身的性质。也可以研究稍微不同的问题,即找寻 $\boldsymbol{\omega}, \boldsymbol{\mu}, f$ 应满足的条件,使得它们意味着对小的 ε,存在不变圆环面,其谱依赖于 ε,但在某个适当的意义下是接近于存在的 $\boldsymbol{\omega}$。

关于上述内容有大量的文献,但客观地说,特别就惟一性和解析性来说,形势依然不是令人满意。欲知更多内容,请读者参阅 Gallavotti et al. (2004)。

相空间里的扩散

KAM 定理意味着一个对非等时解析的可积系统的扰动,即有一个解析的哈密顿量 $\mathcal{H}_\epsilon(\boldsymbol{A},\boldsymbol{\alpha})=\mathcal{H}_0(\boldsymbol{A})+\epsilon f(\boldsymbol{A},\boldsymbol{\alpha})$,其非退化的黑斯矩阵 $\partial^2_{\boldsymbol{AA}}h(\boldsymbol{A})$ 产生了一个大的最大不变圆环面的族。这样的圆环面处于能量面上,但是在其上并没有余维数 1,即它们不把为 $(2\ell-1)$ 维的能量面分裂成非连通的区域,当然,两自由度的系统是例外(见"准周期性与 KAM 稳定性"一节)。

所以,必存在这样的轨道,其在作用量空间接近 $\boldsymbol{A}^i$ 的初始条件,对不管多小的 $\epsilon\neq0$,会到达相空间接近 $A^f\neq A^i$ 的值。尽管相应的轨道必须在一个空间中运行,此空间中在每个 $\{\boldsymbol{A}\}\times\mathbb{T}^\ell$ 附近,有一个不变的表面,其上的点的运动保持 $\boldsymbol{A}$ 在 $O(\epsilon)$ 范围(对小的 ϵ,这个范围可能 $\ll|A^f-A^i|$)内不变,这样的扩散现象依然会发生。

在一个 $s_1=1,s_2=0$ 的先验不稳定的系统中(参见"共振及其稳定性"一节),不难看出相应的现象确实会发生:范例(Arnol′d)就是如下的先验不稳定系统

$$\mathcal{H}_\epsilon=\frac{A_1^2}{2}+A_2+\frac{p^2}{2}+g(\cos q-1)+\epsilon(\cos\alpha_1+\sin\alpha_2)(\cos q-1) \qquad [90]$$

这是一个描述同"转轮"((A_1,α_1) 坐标系)和"时钟" ((A_2,α_2) 坐标系)相互作用的"单摆"运动((p,q) 坐标系)的系统,此运动在点 $p=0,q=0,2\pi$ ($s_1=1,s_2=0,\lambda_1=\sqrt{g}$,比较式[86])附近是先验不稳定的。可以证明,在能量面 E 上,对任意足够小的(不管多小)$\epsilon\neq0$,有初始值,其作用量坐标接近 $\boldsymbol{A}^i=(A_1^i,A_2^i)$,而 $(1/2){A_1}^{i2}+{A_2}^{i2}$ 接近 E,会最终演化入某个值 $A'=(A_1',A_2')$,A_1' 同 ${A_1}^f$ 的距离小于任意事先设定的值(当然具有能量 E)。进一步,整个过程中单摆的能量总是保持在 $O(\epsilon)$ 范围内接近于零(即单摆的摆动在未扰动的分隔线附近)。

换句话说,式[90]描述的是一架机器(单摆)近似的在一个循环内期内工作,从一个库(时钟)中提取能量然后把能量传递给一个机械部件(轮子)。扩散是可能的意思是,如果作为 ϵ 函数的初始作用量和初始相位(即 α_1,α_2,p,q)调节得合适,则只要 $\epsilon\neq0$ 装置就能工作。

系统[90]的特别之处是未扰动系统的固定点 $P_\pm$(即平衡点 $p=0,q=0,2\pi$),即使 $\epsilon\neq0$,仍保持是不稳定的平衡点,这是一个重要的可用于简化问题的特征。

这个特别之处允许我们在分析更一般的问题时能绕过障碍。障碍指由满足 $\boldsymbol{A}_1\boldsymbol{v}_1+\boldsymbol{A}_2\boldsymbol{v}_2=0$ 的 $\boldsymbol{A}$ 组成的共振能量面,对应于在扰动函数中出现的谐波 $(\boldsymbol{v}_1,\boldsymbol{v}_2)$。这些谐波在用接近 $\boldsymbol{A}$ 的作用量构造扰动不变圆环面的参数方程(用 Arnol′d 方法研究[90]时需用到)时会引起除以零的操作。在式[90]中,问题都处在图 6 中的粗线所表示的共振上,即 $A_1=0$,对应式[90]中的 $\cos\alpha_1$。

如果 $\epsilon=0$,点 P_- $(p=0,q=0)$ 和点 P_+ $(p=0,q=2\pi)$ 都是非稳定的平衡点(当然,如果 q 是角变量,这两个点是同一个点)。P_+ 的非稳定流形(是条曲线)和 P_- 的稳定流形重合,反之亦然。所以,未扰动系统在双无穷大的时间间隔 $(-\infty,+\infty)$ 内有非平凡的从 P_+ 到 P_- 和从 P_- 到 P_+ 的运动:变量 p,q 描述一个单摆,而 $P_\pm$ 是它的由分隔曲线[①]相连接的非稳定平衡点。

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① 构成单摆的零-能量面,即周期性轨道和发散轨道的分界线——译者注。

对于更一般的先验不稳定哈密顿量

$$\left.\begin{aligned}&\mathcal{H}_\epsilon = \mathcal{H}_0(\boldsymbol{A}) + \mathcal{H}_u(p,q) + \epsilon f(\boldsymbol{A},\boldsymbol{\alpha},p,q)\\&\text{in } (U\times\mathcal{T}^l)\times(\mathcal{R}^2)\end{aligned}\right\} \qquad [91]$$

上述性质也成立。这里 $\mathcal{H}_u$ 是一维的哈密顿量,有在一个方向上线性相斥而在另一个方向上线性吸引的两个非稳定的平衡点 P_+ 和 P_-,它们由两个异宿的轨道相联系,当时间趋于$\pm\infty$时,趋近点 P_+ 和 P_-,或者反过来。

实际上,(固定)点无需是不同的,但如果重合,连接它们的轨道必须是非平凡的。式[90]中变量 q 可当作一个角变量,则 P_+ 和 P_- 会重合(但由非平凡的轨道相连接,即也经过除 $P_\pm$ 以外的其他点的轨道)。这样的轨道,如果 $P_+\neq P_-$,称为异宿的;若 $P_+=P_-$,则称为同宿的。

一般情况下,除了同宿(或异宿)条件外,必须添加一些式[90]自动满足的弱一般性条件,使得给定的其未扰动能量为 E 的 $\boldsymbol{A}^i$ 和 $\boldsymbol{A}^f$,对于足够小但不等于零的 ϵ,能找到作用量任意接近 A^i 的初始值(依赖于 ϵ)并演化到作用量任意接近 $\boldsymbol{A}^f$ 的值。此现象被称为**Arnol′d 扩散**。从 $\boldsymbol{A}^i$ 附近到 $\boldsymbol{A}^f$ 附近的过渡的简单充分条件表述如下:

定理 7 给定式[91]的哈密顿量,而 $\mathcal{H}_u$ 有两个通过异宿轨道,$t\to(p_a(t),q_a(t))$,$a=1,2$,连接的双曲固定点 $P_\pm$,假设

(i)在能量为 $E=\mathcal{H}(\boldsymbol{A}^i)+\mathcal{H}_u(P_\pm)$ 的未扰动能量面上有正则的连接 $\boldsymbol{A}^i$ 到 $\boldsymbol{A}^f$ 的曲线 $\gamma:s\to\boldsymbol{A}(s)$,使得未扰动的圆环面 $\{\boldsymbol{A}(s)\times\mathbb{T}^l\}$,在 $\epsilon\neq0$ 附近,对于填充曲线 γ 而只剩下量级为 $O(\epsilon)$ 的缝隙的集合对应的 s,可以延拓到不变圆环面 $T_{A(s),\epsilon}$。

(ii)函数 f 对异宿运动的积分的二阶导数 $\boldsymbol{D}_{ij}$,一个 $l\times l$ 矩阵,是非退化的,即对所有的在曲线 γ 上的 $\boldsymbol{A}$ 和所有的 $\boldsymbol{\alpha}\in\mathbb{T}^2$,有

$$|\det\boldsymbol{D}| = \left|\det\left(\int_{-\infty}^{+\infty} dt\,\partial_{\alpha_i\alpha_j} f(\boldsymbol{A},\boldsymbol{\alpha}+\boldsymbol{\omega}(\boldsymbol{A})t,p_a(t),q_a(t))\right)\right| > c > 0 \qquad [92]$$

则给定任意的 $\rho>0$,对足够小的 $\epsilon\neq0$,存在其作用量和能量比 ρ 更接近 $\boldsymbol{A}^i$ 和 E 的初始值,在足够长的时间以后会获得比 ρ 更接近 $\boldsymbol{A}^f$ 的作用量(保持初始能量不变)。

可以证明,上述两个条件,如果自由度$\geqslant3$,对许多 $\boldsymbol{A}^i\neq\boldsymbol{A}^f$(以及许多连接它们的曲线 γ)是成立的。所以,Arnol′d 原先讨论范例[90]的论证经简单推广后就可以证明先验非稳定系统中扩散的存在性。式[92]中的积分称为 Melnikov 积分。

真正的困难在于估计过渡所需的时间,很明显此时间当 $\epsilon\to0$ 时是发散的。假设 g 是固定的(即不依赖于 ϵ 的),朴素的做法很容易就得到比 $O(\exp(a\epsilon^{-b}))$(对某些 $a,b>0$)更糟糕的估计。最终可以看到,在这种情况下,对一般的扰动 $\epsilon f(\boldsymbol{\alpha},q)$,最小的时间估计为 $O(\epsilon^{-1}\lg\epsilon^{-1})$,这是一般性的假设下能期望的最好结果了。

欲知更多的细节,读者可参阅 Arnol′d(1989) 和 Chierchia, Vladinoci(2000)。

准周期运动的长时稳定性

更难的问题是,作用量空间里的同一迁徙现象在先验稳定的系统中是否也会出现?困难的根本在于准周期运动相当稳定的特性。考虑哈密顿量 $\mathcal{H}_\epsilon(\boldsymbol{A},\boldsymbol{\alpha})=\boldsymbol{h}(\boldsymbol{A})+\epsilon f(\boldsymbol{A},\boldsymbol{\alpha})$,$\mathcal{H}_0(\boldsymbol{A})=h(\boldsymbol{A})$在一个开的、有界区域 $U\subset\mathbb{R}^l$ 的闭包 $\bar{U}$ 上是严格凸的、解析的、非等时,扰动$\epsilon f(\boldsymbol{A},\boldsymbol{\alpha})$在 $\bar{U}\times\mathbb{T}^l$中是解析的。

可得到从接近 $\boldsymbol{A}_1$ 的作用量到接近 $\boldsymbol{A}_2$ 的作用量迁徙所需的时间之先验的界限,此界限当 $\varepsilon\to 0$ 时是指数型的(即其下界的行为如同一个 ε 的倒数幂的指数函数)。最简单的定理(Nekhorossev)如下:

定理 8 存在常数 $0<a,b,d,g,\tau$,使得任意初始值 $(\boldsymbol{A},\boldsymbol{\alpha})$ 的演化结果为,在以 $\tau\exp(b\varepsilon^{-d})$ 为上界的时间内,A 的变化不大于 $a\varepsilon^{g}$。

因此,这为扩散的时间设定了一个指数型的上界,即一个 ε 倒数的幂的指数函数确定的上界。在 $\tau\exp(b\varepsilon^{-d})$ 的时间内,作用量的变化为 $O(\varepsilon^{g})$ 量级,所以不管 $\varepsilon\neq 0$ 多小,这个变化都不会大。这就为先验稳定系统的扩散时间设定了一个上界。

对此定理的证明实际上会提供作用量变化的有趣的图像细节,有些作用量比别的作用量的变化要慢得多。

上述定理是构造性的,即所有的常数 $0<a,b,d,\tau$ 都可以显性地选择为依赖于 $I,\mathcal{H}_0,f$,尽管有的也可以选择为只依赖于 I 和 $\mathcal{H}_0$ 的凸图的最小曲率。上述证明可以加以改造从而适应于不属于有严格凸的未扰动哈密顿的系统,甚至是共振未扰动的情形。

但是,在一些重要问题(比如,天体力学中常见的三体问题)上,经验表明,扩散过程很快(即不是前述的指数型的缓慢),同时若应用上述结果,相空间中的快速迁徙是不允许的。然而,对于这些问题上述定理的前提是不成立的,因为未扰动的系统是强烈共振的(一如在天体力学问题中,独立的频率数占自由度数的一部分,而 $h(\boldsymbol{A})$ 远不是严格凸的),这对观察到快速扩散留有广泛的可能性。

进一步,改变假设将大大地变动结果。举例来说,有时可以证明存在快速扩散,虽然也可能需要指数型的长时间。已知的例子是一个三时间尺度的体系,其哈密顿量为

$$\boldsymbol{\omega}_1 A_1+\omega_2 A_2+\frac{p^2}{2}+g(1+\cos q)+\varepsilon f(\alpha_1,\alpha_2,p,q) \qquad [93]$$

$\boldsymbol{\omega}_\varepsilon \overset{\text{def}}{=}(\omega_1,\omega_2)$,$\omega_1=\varepsilon^{1/2}\bar{\omega}$,$\omega_2=\varepsilon^{-1/2}\tilde{\omega}$,而 $\bar{\omega},\tilde{\omega}>0$ 是常数。3 个时间尺度是 ω_1^{-1},$\sqrt{g^{-1}}$,ω_2^{-1}。这种情况下,有许多(虽然不是全部)成对的 $\boldsymbol{A}_1,\boldsymbol{A}_2$ 可以在估计是 $O(\varepsilon^{-1}\lg\varepsilon^{-1})$ 量级的时间内连接起来。

这是不满足条件[92]的一个先验不稳定系统中的快速扩散的例子,因为依赖于 ε 的 $\boldsymbol{\omega}(\boldsymbol{A})$ 意味着[92]中的下限 c 也依赖于 ε(当 $\varepsilon\to 0$ 时,它是 ε 的倒数幂的指数那样的小)。

未扰动系统[93]中 $\mathcal{H}_0$ 的部分对在一个零测度的集合之外(即矢量 $\boldsymbol{\omega}_\varepsilon$ 满足一个适当的丢番图性质)的 $\varepsilon>0$ 是非共振的,且是先验非稳定的,实际应用中遇到的情况 $\mathcal{H}_0$ 的部分可以是先验稳定的和共振的(但经常是非等时的)。对这样的系统,不仅对扩散的速度未能很好地理解,就是证明其存在性的建议,如果有,到目前为止也没能给出令人满意的结果。

欲知更多的细节,读者可参阅 Nekhorossev(1977)。

三体问题

力学几乎等同于三体问题。这样说是因为 3 个通过引力相互作用的质点的运动一直以来都是天文学关键问题,同时也是许多技术的灵感来源,其中最重要的是扰动理论。

作为导论,考虑一个特例。令 3 个质量体,$m_S=m_0$,$m_J=m_1$,$m_M=m_2$,通过引力相互作用,即相互作用势为 $-km_im_j|x_i-x_j|^{-1}$。最简单的情形为第三个物体的质量相对于

另外两个忽略不计,而那两个质量体在一个圆形轨道上运动。进一步,令 $m_J=\varepsilon m_S$,ε 是一小量,质点 m_M 在圆形轨道所在的平面上运动。这是所谓的"圆形限制的三体问题"。

在一个以 S 为中心,绕 S 以角速率 J 转动的参考系里,惯性力(向心力和科里奥利力)起作用。假设质点 J 处在以 $\boldsymbol{i}$ 为单位矢量的轴上,离原点 S 的距离为 R,则质点 M 的加速度为

$$\ddot{\boldsymbol{\rho}}=\boldsymbol{F}+\boldsymbol{\omega}_0^2\left(\boldsymbol{\rho}-\frac{\varepsilon R}{1+\varepsilon}\boldsymbol{i}\right)-2\boldsymbol{\omega}_0\wedge\dot{\boldsymbol{\rho}}$$

如果 $\boldsymbol{F}$ 是吸引力,$\boldsymbol{\omega}_0\wedge\dot{\rho}\equiv\boldsymbol{\omega}_0\dot{\rho}^{\perp}$,这里 $\boldsymbol{\omega}_0$ 是垂直于轨道平面的矢量,$|\boldsymbol{\omega}_0|=\omega_0$;如果 $\rho=(\rho_1,\rho_2)$,则 $\rho^{\perp}\overset{\text{def}}{=}(-\rho_2,\rho_1)$。考虑到原点 S 绕固定的质心转动,$\boldsymbol{\omega}_0^2(\rho-\varepsilon R/(1+\varepsilon)\boldsymbol{i})$ 是向心力,而 $-2\boldsymbol{\omega}_0\wedge\dot{\rho}$ 是科里奥利力。运动方程可以由拉格朗日量得到,拉格朗日量为

$$\mathcal{L}=\frac{1}{2}\dot{\rho}^2-W+\omega_0\rho^{\perp}\cdot\dot{\rho}+\frac{1}{2}\omega_0^2\rho^2-\omega_0^2\frac{\varepsilon R}{1+\varepsilon}\rho\cdot\boldsymbol{i}\qquad[94]$$

和

$$\boldsymbol{\omega}_0^2R^3=km_S(1+\varepsilon)\overset{\text{def}}{=}g_0$$

$$W=-\frac{km_S}{|\rho|}-\frac{km_S\varepsilon}{|\rho-R\boldsymbol{i}|}$$

其中,k 是引力常数,R 是 S 和 J 之间的距离,式[94]中的最后 3 项来自科里奥利力(第一项)和向心力(其他两项,考虑了原点 S 绕固定的质心转动)。

令 $g=g_0/(1+\varepsilon)\equiv km_S$,系统的哈密顿量为

$$\mathcal{H}=\frac{1}{2}(\boldsymbol{p}-\boldsymbol{\omega}_0\rho^{\perp})^2-\frac{g}{|\rho|}-\frac{1}{2}\boldsymbol{\omega}_0^2\rho^2-\varepsilon\frac{g}{R}\left(\left|\frac{\rho}{R}-\boldsymbol{i}\right|^{-1}-\frac{\rho}{R}\cdot\boldsymbol{i}\right)\qquad[95]$$

第一部分可以马上用两体问题的作用量-角坐标来表示(比较"牛顿势与开普勒定律"一节)。记这样的作用量-角坐标为 $(L_0,\lambda_0,G_0,\gamma_0)$,令 θ_0 为 M 相对于椭圆主轴的极角,λ_0 为 M 在椭圆上的平均偏角,考虑到 $\varepsilon=0$,椭圆的轴以速度 $-\omega_0$ 转动,哈密顿量变为

$$\mathcal{H}=-\frac{g^2}{2L_0^2}-\boldsymbol{\omega}_0G_0-\varepsilon\frac{g}{R}\left(\left|\frac{\rho}{R}-\boldsymbol{i}\right|^{-1}-\frac{\rho}{R}\cdot\boldsymbol{i}\right)\qquad[96]$$

这对研究内部的问题,即 $|\rho|<R$,会很方便。可以通过式[41],式[42]用作用量-角表达

$$\left.\begin{aligned}&\theta_0=\lambda_0+f_{\lambda_0},\qquad\theta_0+\gamma_0=\lambda_0+\gamma_0+f_{\lambda_0}\\&e=\left(1-\frac{G_0^2}{L_0^2}\right)^{1/2},\frac{|\rho|}{R}=\frac{G_0^2}{gR}\frac{1}{1+e\cos(\lambda_0+f_{\lambda_0})}\end{aligned}\right\}\qquad[97]$$

这里(见式[42])$f_\lambda=f(e\sin\lambda,e\cos\lambda)$,且有

$$f(x,y)=2x\left(1+\frac{5}{4}y+\cdots\right)$$

省略号代表 x,y 的高阶项。如果 $\omega^2=gR^{-3}$,哈密顿量的形式为

$$\mathcal{H}_\varepsilon=-\frac{g^2}{2L_0^2}-\omega G_0+\varepsilon\frac{g}{R}F(G_0,L_0,\lambda_0,\lambda_0+\gamma_0)\qquad[98]$$

惟一重要的特性(对我们这里的讨论来说)是,$F(L,G,\alpha,\beta)$ 在满足 $|G|<L$,$|\rho|<R$ 的某点的邻域内之关于 L,G,α,β 是解析函数。但是,关于 G 的解析域非常小,被限制在 $|G|<L$,因而就排除了圆形轨道的特例 $G=\pm L$。

注意,KAM 定理看起来好像不适用于式[98],因为 $\mathcal{H}_0(L,G)$ 的二阶微分矩阵的值为零。但是,只要稍加修订,定理的证明能通过这一关。这可以通过推敲证明过程加以验证,或如庞加莱那样,简单地注意到"平方"哈密顿量 $\mathcal{H}'_\epsilon \equiv (\mathcal{H}_\epsilon)^2$ 的形式为

$$\mathcal{H}'_\epsilon = \left(-\frac{g^2}{2L_0^2} - \omega G_0\right)^2 + \varepsilon F'(G_0, L_0, \lambda_0, \lambda_0 + \gamma_0) \qquad [99]$$

其中 F' 是解析的。但此时如果 $h = -g^2 L_0^{-2} - 2\omega G_0 \neq 0$,则

$$\det \frac{\partial^2 H'_0}{\partial(G_0, L_0)} = -6g^2 L_0^{-4} \omega_0^2 h \neq 0$$

所以 KAM 定理适用于 $\mathcal{H}'_\epsilon$。关键是 $(\mathcal{H}_\epsilon)^2$ 所产生的轨道和 $\mathcal{H}_\epsilon$ 所产生的轨道几何上是相同的,它们只是因为一个时间标度常数因子 $2H_\epsilon$ 而速度不同罢了。

这表明,给定一未扰动的椭圆,其参数为 (L_0, G_0),其中 $\omega = (g^2/L_0^3, -\omega)$,$G_0 > 0$,且 ω_1/ω_2 是丢番图的,则如果 ε 足够小,受扰动系统的运动是谱正比于 ω 的准周期运动,发生在绕一个永远保持在未扰动圆环面(作用量为 (L_0, G_0))附近之圆环面的轨道上(可视作描述一个根据面积定理在一个转动速率为 $-\boldsymbol{\omega}_0$ 的椭圆上的点的运动)。因此,KAM 定理至少从概念上回答了下面的经典问题:一个三体问题的解会永远停留在未扰动的运动附近吗?即太阳系可能永远是稳定的吗?

假设 $e, |\rho|/R \ll 1$,且保留关于 e 和 $|\rho|/R \ll 1$ 的最小阶,哈密顿量[98]简化为

$$\mathcal{H} = -\frac{g^2}{2L_0^2} - \omega G_0 + \delta_\epsilon(G_0) - \varepsilon \frac{g}{2R} \frac{G_0^4}{g^2 R^2} (3\cos 2(\lambda_0 + \gamma_0) - e\cos\lambda_0 - \frac{9}{2} e\cos(\lambda_0 + 2\gamma_0) + \frac{3}{2} e\cos(3\lambda_0 + 2\gamma_0)) \qquad [100]$$

其中

$$\delta_\epsilon(G_0) = -((1+\epsilon)^{1/2} - 1)\omega G_0 - \varepsilon \frac{g}{2R} \frac{G_0^4}{g^2 R^2}$$

$$e = \left(1 - \frac{G_0^2}{L_0^2}\right)^{1/2}$$

可以以哈密顿量[100]为模型,循着 KAM 的证明,当作一个有趣的练习来估计 ε 要多小时,一个行星(取水星的数据,作用量可取现在的值)在一个质量为 ε 乘上太阳质量的物体——其在离太阳的距离为太阳-木星之间的距离的圆形轨道上运动——的影响下,其在一个(缓慢进动)的轨道上会永远是稳定的。这个问题即可以循着上述约化到通常的 KAM 定理的做法,也可以循着"准周期性与 KAM 稳定性"一节中的途径,直接对式[100]应用 Lindestedt 级数展开。第一种方法较容易,但第二种方法更有效;但是除非特别仔细进行估计,否则得到的值 ϵm_S 从天文学的观点来看是无意义的。

欲知更多的细节,读者可参阅 Arnol′d(1989)。

奇点的有理化和正则化

可积系统经常会有一些有趣的初始值处于可积域的边界之外。例如,当 $L=G$ 时的有心运动(圆形轨道)或刚体绕一个主轴转动,或是 $G=0$ 时的两体运动(碰撞)。在这些情形下,上述讨论过的摄动理论不能应用。典型的扰动依赖于像 $\sqrt{L-G}$ 这样的量,在 $L=G$ 处不是解析的。但是,有时可以扩大相空间,在原来的相空间是奇点的初始值附近

引入新的坐标。

一个著名的例子是分析圆形限制的三体问题的失败,看起来好像我们要扰动的轨道是圆形时,导致失败。

引入正则坐标系 L,λ 和 G,γ 是方便的,

$$\left.\begin{aligned} L &= L_0, \qquad G = L_0 - G_0 \\ \lambda &= \lambda_0 + \gamma_0, \qquad \gamma = -\gamma_0 \end{aligned}\right\} \tag{101}$$

使得 $e=\sqrt{2GL^{-1}}\sqrt{1-G(2L)^{-1}}$,且有 $\lambda_0=\lambda+\gamma,\theta_0=\lambda_0+f_{\lambda_0}$,$f_{\lambda_0}$ 在式[42]中定义(见式[97])。所以,

$$\left.\begin{aligned} &\theta_0 = \lambda+\gamma+f_{\lambda+\gamma} \qquad \theta_0+\gamma_0 = \lambda+f_{\lambda+\gamma} \\ &e = \sqrt{2G}\sqrt{\frac{1}{L}\left(1-\frac{G}{2L}\right)} \\ &\frac{|\rho|}{R} = \frac{L^2(1-e^2)}{gR}\,\frac{1}{1+e\cos(\lambda+\gamma+f_{\lambda+\gamma})} \end{aligned}\right\} \tag{102}$$

而哈密顿量[100]的形式为

$$\mathcal{H}_\epsilon = -\frac{g^2}{2L^2} - \omega L + \omega G + \epsilon\frac{g}{R}F(L-G,L,\lambda+\gamma,\lambda) \tag{103}$$

在式[101]的 L,G 坐标系里,未扰动的圆周运动对应于 $G=0$,且式[96]一旦用作用量-角变量 G,L,γ,λ 表示,它就是在一个大小由 $\sqrt{G}$ 控制的区域内是解析的。进一步,摄动理论常常可以加以正则化。

这可以通过在奇点(坐标域的边界点)周围增加点(一个或多个),并用新的坐标系同时描述奇点附近的点以及新加的点的方式"扩展可积性"区域。在许多有趣的情形下,运动方程在新坐标系下不再是奇异的(即变成解析的了),因此可恰当地用来描述在有限时间内到达奇点的运动。我们可以说原来的奇性只是表观的。

也许在前述的圆周限制的三体问题中这一点可以得到最好的体现,奇性发生在 $G=0$,即在圆形的未扰动轨道上。如果我们在新坐标系中用 G 为小值描述这些点,该新坐标系通过式[101]得到,即保留 L,λ,并令

$$p = \sqrt{2G}\cos\gamma, \quad q = \sqrt{2G}\sin\gamma \tag{104}$$

则 p,q 在原点的邻域——但不包括原点——内变化。

在 p-q 平面加入原点后,则在原点的全部邻域内哈密顿量[96]关于 L,λ,p,q 是解析的。这是因为它作为 L,λ 和 $e\cos\theta_0,\cos(\lambda_0+\theta_0)$ 的函数是解析的(比较式[96]和式[97])。因为由式[97],$\theta_0=\lambda+\gamma+f_{\lambda+\gamma}$ 及 $\theta_0+\lambda_0=\lambda+f_{\lambda+\gamma}$,哈密顿量[96]对于小的 e(即小的 G)关于 $L,\lambda,e\cos(\lambda+\gamma+f_{\lambda+\gamma})$,$e\cos(\lambda+f_{\lambda+\gamma})$ 是解析的;且由式[42]有 $f_{\lambda+\gamma}$ 关于 $e\sin(\lambda+\gamma)$ 和 $e\cos(\lambda+\gamma)$ 是解析的。因此,下面的三角恒等式

$$\begin{aligned} e\sin(\lambda+\gamma) &= \frac{p\sin\lambda+q\cos\lambda}{\sqrt{L}}\sqrt{1-\frac{G}{2L}} \\ e\cos(\lambda+\gamma) &= \frac{p\cos\lambda-q\sin\lambda}{\sqrt{L}}\sqrt{1-\frac{G}{2L}} \end{aligned} \tag{105}$$

同 $G=(1/2)(p^2+q^2)$ 一起保证式[103]在 $p=q=0$ 和 $L>0,\lambda\in[0,2\pi]$ 附近是解析的。哈密顿量

变成解析的,新的坐标系适于描述过原点的运动。举例来说,令 $C\overset{\text{def}}{=}\frac{1}{2}\left(1-\frac{p^2+q^2}{4L}\right)L^{-1/2}$,式[100]变成

$$H=-\frac{g^2}{2L^2}-\omega L+\omega\frac{1}{2}(p^2+q^2)+\delta_\varepsilon\left(\frac{1}{2}(p^2+q^2)\right)-\varepsilon\frac{g}{2R}\frac{\left(L-\frac{1}{2}(p^2+q^2)\right)^4}{g^2R^2}$$
$$\times(3\cos2\lambda-((-11\cos\lambda+3\cos3\lambda)p-(7\sin\lambda+3\sin3\lambda)q)C) \qquad [106]$$

上面讨论的 KAM 定理没有应用于"笛卡儿坐标系",即如式[106],未扰动系统没有用作用量-角坐标表示。然而,有些该定理的版本(实际是它的引理)是可应用的,因此有可能利用这里所述的技术得到一些甚至是关于圆周运动扰动的结果。

类似的,对绕固定点的置于解析的力场之下的刚体的哈密顿量,当其运动是接近绕某个主轴的转动,或更一般地,是接近某个轴 i_3,z 或 z_0 中的任何两个重合(即在主轴、角动量轴和惯量 z 轴中任意两个重合,见"刚体"一节)那样的构型时,如果用 Deprit 作用量-角描述,它是奇异的。但是,仿照针对圆周三体问题那样简单情形所描述的程序,可以扩展其相空间使得用新坐标写成的哈密顿量在奇异构型附近是解析的。

当考虑不受任何限制的平面内三体问题的碰撞轨道时,也有正则化的问题。在这方面,一个引人注目的结果是平面三体问题碰撞轨道的正则化。在证明了如果总角动量不为零,三体同时碰撞在任何有限时间间隔内不会发生后,问题约化为在总角动量不为零的前提下两体碰撞的正则化。

把两个碰撞体的相对位置坐标(x,y)做改变$(x,y)\to(\xi,\eta)$,$x+iy=(\xi+i\eta)^2$,这样的局域坐标变换不是一对一的,因此如果不同(ξ,η)对应的点可看作是不同的,则可以看作是对位置空间的拓展。但用变量 ξ,η 写成的运动方程在 $\xi,\eta=0$ 处没有奇点(Levi-Civita)。

另一个著名的例子是对 Schwartzshild 度规的正则化,即两体问题的广义相对论版本。此问题有些超出本评论的范围(Synge,Kruskal)。

欲知更多的细节,读者可参阅 Levi-Civita(1956)。

附录一:KAM 求和规则

控制"剩余贡献"的想法是要把问题约化为这样的情形,在树结构中不存在相连的一对连线,其上的流相等。把树图(见式[74]和式[83])上除数为 $C/\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l)>1$ 的线加上 0 尺度标记,这些是在估计时不会引起问题的连线。然后,把流为 $\boldsymbol{v}(l)$,且 $|\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l)|\leqslant 2^{-n+1}$,$n=1$ 的连线(此即是剩余连线)加上尺度标记 $\geqslant 1$。

带标记 0 的连线说成是 0 尺度的,标记为$\geqslant 1$ 的说成是尺度$\geqslant 1$ 的。一个 0 尺度的团簇是树 θ 中形成一个连通子图的所有 0 尺度的连线的最大集。

考虑树族 Θ_0 中不包含 0 尺度的连线的团簇,只有携带相同的流的一根进入和一根离开团簇的连线的树 $\theta_0\in\Theta_0$。

引入居于连线 l',$l(l'>l)$中间的连线记号 l_1 是有益的,它意味着 l_1 在 l' 之前,但不在 l 之前。

包含一些尺度标记$\geqslant 1$ 的(其上流相等的)且其间所有连线的尺度标记都为 0 的相邻连线对 $l'>l$ 的所有树 θ,都可以通过下述方式构造:可在标记$\geqslant 1$ 的树族 Θ_0 的连线上插入任

何数目的连线团簇和结点,具有 0 尺度标记的连线,且要求插入的节点的谐波之和为零。

考虑一条连接节点 $v_1<v_2$,标尺$\geqslant 1$ 的连线,$l_0\in\theta_0\in\Theta_0$。设想在其中插入一个 0 尺度的连线的簇 γ,所有的节点谐波之和为零,且从其中引出一根线连接 γ 中的节点 v_{out} 到 v_2,另一根线连接 γ 中的节点 v_{in} 到 v_1。插入 k 连线,$|\gamma|=(k+1)$ 节点的簇会通过替换线因子,也简称为"团簇 γ 的值",改变树图的值。线因子被替换为

$$\frac{\boldsymbol{v}_{v_1}\cdot\boldsymbol{v}_{v_2}}{\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l_0)^2}\to\frac{(\boldsymbol{v}_{v_1}\cdot\boldsymbol{M}(\gamma;\boldsymbol{v}(l_0))\boldsymbol{v}_{v_2})}{\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l_0)^2}\frac{1}{\omega_0\cdot v(l_0)^2}\qquad[107]$$

这里的 $\boldsymbol{M}$ 是一个 $l\times l$ 矩阵,如果 $l=v'v$ 表示 v' 和 v 之间的连线,则

$$\boldsymbol{M}_{rs}(\gamma,\boldsymbol{v}(l_0))=\frac{\epsilon^{|r|}}{k!}v_{\text{out},r}v_{\text{in},s}\prod_{v\in\gamma}(-f_{v_v})\prod_{l\in\gamma}\frac{\boldsymbol{v}_v\cdot\boldsymbol{v}_{v'}}{\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l)^2}$$

因此,如果各种可能的连通团簇都插入,所得到的树的值可以通过相加得到,即通过赋予原来的连线 l_0 一个类似式[107]的因子,但是用 $\boldsymbol{M}^{(0)}(\boldsymbol{v}(l_0))\overset{\text{def}}{=}\sum_\gamma\boldsymbol{M}(\gamma;\boldsymbol{v}(l_0))$ 替代 $\boldsymbol{M}(\gamma;v(l_0))$ 而得到。

如果几个连通的团簇 γ 都插入在同一条线上,求它们值的和等价于把连线 l_0 的因子修改为

$$\begin{aligned}&\sum_{k=0}^{\infty}\boldsymbol{v}_{v_1}\cdot\left(\frac{\boldsymbol{M}^{(0)}(\boldsymbol{v}(l_0))}{\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l_0)^2}\right)\boldsymbol{v}_{v_2}\frac{1}{\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l_0)^2}\\&=\left(\boldsymbol{v}_{v_1}\cdot\frac{1}{\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l_0)^2-\boldsymbol{M}^{(0)}(\boldsymbol{v}(l_0))}\boldsymbol{v}_{v_2}\right)\end{aligned}\qquad[108]$$

定义 $\boldsymbol{M}^{(0)}$ 的级数,由其构造可知,只涉及 0 尺度连线的树,因此有大的除数,所以若 ϵ 足够小,它收敛于一个 ϵ 量级(更确切地,是 ϵ^2)的小尺度矩阵。

收敛性可简单地如下确立:因为定义 $\boldsymbol{M}^{(1)}$ 的级数由传播子值$>(1/2)$的连线构成,所以对于足够小的 ϵ 它当然收敛(在"扰动函数"一节中的估计中,传播子全部为 1),且其和是 ϵ 量级(确切点,是 ϵ^2)的,所以<1。但是,在处理小传播子的连线时不能采用上述的论证(这仍有待讨论)。在考虑尺度大于 1 的连线的时候,最终还是要用到不依赖于传播子大小的方法,很快我们会发现这是有必要的。

由式[108]获得的求和的益处是:我们可以把 $\boldsymbol{h}$ 表述为不同值的树的和,这些树是简单的,因为它们不包含尺度$\geqslant 1$,且中间有 0 尺度的、节点谐波之和为 0 的连线的对。代价是更多地涉及除数,且我们还有未证明式[108]中的级数是收敛的这一问题。实际上,这是个几何级数,其值由式[79]的求和规则得到的结果为式[108]的右边,除非我们能证明几何级数中的比<1[①]。由前述论证可知这是平凡的,但应该知道还有另一个收敛的原因,这里没有必要用到它,但后来会变得重要起来。

几何级数中的比<1 的性质可以看作是"准周期性与 KAM 稳定性"一节介绍过的项抵消的结果,比<1 是因为 $\boldsymbol{M}^{(0)}(\boldsymbol{v}))=\epsilon^2(\boldsymbol{\omega}_0\cdot\boldsymbol{v})^2m^{(0)}(v)$,且对某个 $D_0>0$ 及 $\epsilon_0>0$ 有,$C|m^{(0)}(\boldsymbol{v})|<D_0$(对所有 $|\epsilon|<\epsilon_0$)。因此,对小的 ϵ,式[108]中的除数本质上同开始求和前一样。

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① 译者猜测这里想说的意思是,式[108]的左边是一几何级数,按式[79]求和的结果如式[108]的右边。除非我们能证明几何级数的后项除以前一项<1,[108]左边的级数之收敛性尚未确定。请参阅原文——译者注。

此时,可以开始归纳。考虑用新规则求其值的树,对 $C|\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l)|\leqslant 2^{-n+1}(n=2)$ 的连线加上尺度标记"$\geqslant 2$",已加上标记"0" 连线不变,对其他的连线加上标记"1"。带标记"1"的连线满足 $2^{-n}<|\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l)|\leqslant 2^{-n+1}(n=1)$。这样由构造可知图包含尺度标记为 0,1 或$\geqslant 2$ 的连线,但标记为"$\geqslant 1$"连线不出现。

一个尺度 1 的团簇是树 θ 中形成一个连通子图的所有 0 尺度和 1 的连线的最大集,它至少包括一根标记 1 的连线。

可以重复关于 0 尺度的团簇的构造来考虑树族 $\theta_1\in\Theta_1$,其中 Θ_1 是由包含标记为 0,1 或$\geqslant 2$ 的连线的树的集合,其中且这些树不包含相连的带相同动量的连线对(如果它们之间只有标记为 0 和 1 的连线)。

插入一个这样连线的簇 γ 到 θ_1 中的连线 l_0 上导致定义了一个矩阵 $\boldsymbol{M}^{(1)}$,该矩阵是通过对含标记 0 和 1 的连线(用式[107]定义的连线因子对其赋值)的团簇 γ 的树值求和形成的。这里,γ 被限制为那些不含有流相同的且其间任何连线为低阶(标记为 0)的连线的连线对 $l'<l$ 的 γ,"其间"的意思是在 l' 之前,但不在 l 之前。

所以,有必要发展一个与尺度无关的方法来验证 $\boldsymbol{M}^{(1)}$ 以及后来要引入的处理高阶传播子的矩阵的收敛性。这可以通过扩展"准周期性与 KAM 稳定性"一节中提到的 Siegel 定理来实现。

定理 9 令 $\boldsymbol{\omega}_0$ 满足式[74] 且设 $\boldsymbol{\omega}=C\boldsymbol{\omega}_0$。考虑图 θ 对式[82]中的求和的贡献,而图 θ

(i)没有一对连线 $l'>l$ 处于相同的通往根的路径上携带同样的流 $\boldsymbol{v}$,条件是所有的处于其间的连线 l_1 的流 $\boldsymbol{v}(l_1)$ 满足 $|\boldsymbol{\omega}\cdot\boldsymbol{v}(l_1)|>2|\boldsymbol{\omega}\cdot\boldsymbol{v}|$;

(ii)节点的谐波是有界的,即对某个 N,$|\boldsymbol{v}|<N$,

那么图 θ 中,除数为 $\boldsymbol{\omega}\cdot\boldsymbol{v}_l$,且 $2^{-n}<|\boldsymbol{\omega}\cdot\boldsymbol{v}_l|\leqslant 2^{-n+1}$ 的连线 l 的数目不超过 $4Nk2^{-n/\tau}$,$n=1,2,\cdots$[①]。

这意味着,如式[85]的估计一样,定义 $\boldsymbol{M}^{(1)}$ 的级数收敛。再次,必须验证是否存在抵消,而抵消意味着 $\boldsymbol{M}^{(1)}(\boldsymbol{v}))=\varepsilon^2(\boldsymbol{\omega}_0\cdot\boldsymbol{v})^2 m^{(1)}(\boldsymbol{v})$,而对同样的某个 $D_0>0$ 和同样的 ε_0,有 $|m^{(1)}(\boldsymbol{v})|<D_0$。

此时处理的树只包含带 0,1 和$\geqslant 2$ 连线,且标记为 0 的连线 $l=v'v$ 的线因子为 $\boldsymbol{v}_{v'}\cdot\boldsymbol{v}_v/(\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l))^2$;标记为 1 的连线 $l=v'v$ 的线因子为 $\boldsymbol{v}_{v'}\cdot(\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l)^2-\boldsymbol{M}^{(0)}(\boldsymbol{v}(l)))^{-1}\boldsymbol{v}_v$;标记为$\geqslant 2$ 的连线 $l=v'v$ 的线因子为

$$\boldsymbol{v}_{v'}\cdot(\boldsymbol{\omega}_0\cdot\boldsymbol{v}(l)^2-\boldsymbol{M}^{(1)}(\boldsymbol{v}(l)))^{-1}\boldsymbol{v}_v$$

进一步,没有一对标记为"1"或"$\geqslant 2$"的具有相同的动量且其间只有低阶连线(即第一种情况下只有"0",第二种情况下只有"0"和"1")的连线对是相连接的。

这个计算程序可以迭代,经无穷多步以后,直到问题约化为计算这样的树的值,它的每一个连线的标记为 n,但没有一对是相连接的,且其间的任何连线都是低阶的,则 Siegel 的论证又能应用,这样得到的级数是绝对收敛的,是关于 ε 的解析函数的级数,所以原来的级数是收敛的。

尽管在每一步都有一个分母的下限,且避免使用 Siegel 定理是不可能的。实际上,当尺度增大时,分母会变得越来越糟糕。为了验证对 D_0 和 ε_0 的估计,它们决定各个级数收

① τ 没有定义。原文如此——译者注。

敛性对尺度的独立性,有必要利用上述定理,以及没有必要考虑(每一步)带相同动量的且其间含有高尺度的连线的连线对的特点。

可以对 $h^{(k)}$ 逐阶加上限但不进行重求和(即不改变线因子),且揭示必要的抵消来进行上述的分析。另一种可能是,循着 Kolmogolov, Arnol′d 和 Moser 证明此定理的前 3 个版本(稍有不同)的路径,即对圆环面方程逐阶采取近似。

如同未扰动的圆环面一样,不变圆环面是拉格朗日流形(比较式[31]后面的评论),且当哈密顿量为式[80]时,生成函数 $\boldsymbol{A}\cdot\boldsymbol{\Psi}+\Phi(\boldsymbol{A},\boldsymbol{\Psi})$ 可以用其参数方程表示为

$$\left.\begin{aligned}&\Phi(\boldsymbol{A},\boldsymbol{\Psi})=G(\boldsymbol{\Psi})+a\cdot\boldsymbol{\Psi}+h(\boldsymbol{\Psi})\cdot(\boldsymbol{A}-\boldsymbol{\omega}-\Delta\boldsymbol{h}(\boldsymbol{\Psi}))\\&\partial_{\psi}G(\boldsymbol{\Psi})\overset{\text{def}}{=}-\Delta\boldsymbol{h}(\boldsymbol{\Psi})+\underset{\sim}{h}(\boldsymbol{\Psi})\partial_{\boldsymbol{\psi}}\Delta\underset{\sim}{h}(\boldsymbol{\Psi})-a\\&\boldsymbol{a}\overset{\text{def}}{=}\int(-\Delta\boldsymbol{h}(\boldsymbol{\Psi})+\underset{\sim}{h}(\boldsymbol{\Psi})\partial_{\boldsymbol{\psi}}\Delta\underset{\sim}{h}(\boldsymbol{\Psi}))\frac{\mathrm{d}\boldsymbol{\Psi}}{(2\pi)^{l}}=\int\underset{\sim}{h}(\boldsymbol{\Psi})\partial_{\psi}\Delta\underset{\sim}{h}(\boldsymbol{\Psi})\frac{\mathrm{d}\boldsymbol{\Psi}}{(2\pi)^{l}}\end{aligned}\right\}\quad[109]$$

这里 $\Delta=(\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\psi}})$,不变圆环面对应于映射 $\boldsymbol{\alpha}=\boldsymbol{\Psi}+\partial_{A}\boldsymbol{\Phi}(\boldsymbol{A},\boldsymbol{\Psi})$,$\boldsymbol{A}'=\boldsymbol{A}+\partial_{\boldsymbol{\psi}}\Phi(A,\boldsymbol{\Psi})$ 中的 $\boldsymbol{A}'=\boldsymbol{\omega}$。实际上,由式[109],后一个映射变为 $\boldsymbol{A}'=\boldsymbol{A}-\Delta\boldsymbol{h}$,从只依赖于 $\boldsymbol{\alpha}$ 的 f 之式[75]第二式知,当 $\boldsymbol{A},\boldsymbol{\alpha}$ 在不变圆环面上时,它就是 $\boldsymbol{A}=\boldsymbol{\omega}+\Delta\boldsymbol{h}$。

注意到如果 $\boldsymbol{a}$ 存在,它应由式[109] 中的第三式决定,但是验证式[109]中第二个方程是可解的(即确认右边为某函数的梯度)却不是容易的事。由 $\boldsymbol{A}\cdot\boldsymbol{\Psi}+\boldsymbol{\Phi}(\boldsymbol{A},\boldsymbol{\Psi})$ 生成的正则映射也可以对 $\boldsymbol{\omega}$ 附近的 $\boldsymbol{A}$ 定义,且把不变圆环面的邻域分叶成别的圆环面的叶状结构。当然,对 $\boldsymbol{A}'\neq\boldsymbol{\omega}$ 这样定义的圆环面一般不是不变的。

欲知更多的细节,读者可参阅 Gallavotti et al. (2004)。

附录二:科里奥利力与洛伦兹力——拉莫进动

拉莫进动指的是带电粒子在磁场 $\mathcal{H}$ 中的运动(在惯性参照系内)。它是由于作用在单位质量单位电荷上的洛伦兹力所产生的加速度 $\ddot{\boldsymbol{\rho}}=\boldsymbol{v}\wedge\boldsymbol{H}$ 引起的,这里记光速 $c=1$。

因此,若 $\boldsymbol{H}=H\boldsymbol{k}$ 沿 $\boldsymbol{k}$ 轴方向,如果 $\boldsymbol{H}=2\omega_0\boldsymbol{k}$,则它造成的加速度同在绕 k 轴以角速度 $\omega_0\boldsymbol{k}$ 转动的坐标系中科里奥利力在单位质量上所造成的加速度是一样的。

上述说法意味着,如果 H 和 ω_0 有关系 $H=2\omega_0\boldsymbol{k}$,均匀带单位电荷的绕自身中心自由运动的均质球在沿 k 轴的恒磁场 H 中的运动同没有磁场但是以常角速度为 ω_0 绕 k 轴转动的非惯性坐标系中观察到的一样。在此参考系中,科里奥利力可解释为磁场的作用。

上述说法只当有心力关于中心的力矩为 0 时才成立,球对称情况下当然是这样。在非球对称情况下,有心力的力矩一般不为 0,因此科里奥利力和洛伦兹力的等价只是近似的。

拉莫定理对此有精确的描述。它能定量地给出一般的质量为 m 的粒子的体系在磁场中以及在转动坐标系中的运动的区别。近似程度可由拉莫进动的频率 $eH/2mc$ 的大小来估计(它比系统的其他特征频率要小,其物理意义是有心力要比其他的作用力要小)。

令沿 $\boldsymbol{k}$ 轴方向的恒磁场 $\boldsymbol{H}=2\omega_0\boldsymbol{k}$ 的矢势为 $\boldsymbol{A}$,$\boldsymbol{A}=2\omega_0\boldsymbol{k}\wedge\boldsymbol{\rho}\equiv2\omega_0\rho^{\perp}$。根据“三体问题”一节中(见式[95])对科里奥利力的处理,处于矢势为 $\boldsymbol{A}$ 的磁场 $\boldsymbol{H}$ 中且受势能为 W 的其他力作用的质量为 m,电荷为 e 的粒子,其运动(在惯性坐标系里,用一般的单位,光速为 c)可以用哈密顿量

$$\mathcal{H}=\frac{1}{2m}\left(p-\frac{e}{c}\boldsymbol{A}\right)^2+W(\rho) \qquad [110]$$

描述,其中的 $\boldsymbol{p}=m\dot{\boldsymbol{\rho}}+(e/c)\boldsymbol{A}$ 和 $\boldsymbol{\rho}$ 两者为正则共轭变量。

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导论:微分几何

微分几何是研究诸如曲线、曲面及赋予度量和联络等附加结构的高维流形等几何对象的微分性质。微分几何的一个主要思想是运用分析工具来研究几何问题,特别是研究它们的"无穷小部分",从而使问题线性化。然而,在历史上,几何概念经常超前于从微分几何观点定义它们所需要的分析工具。比如,曲线的切线概念出现在导数概念之前。

尽管微分几何只产生了 200 余年,但它一直强烈地(通常是双向地)影响着物理学。例如,曲线论常用于运动学、辛流形产生于 Hamilton 力学、伪黎曼流形应用于广义相对论、旋量应用于量子力学、李群和主纤维丛应用于规范场理论、无限维流形出现在量子场论的路径积分方法中等。

曲线和曲面

曲线和曲面的微分性质研究起因于坐标法(或解析几何)与无穷小算法的结合,前者由 Descartes 和 Fermat 在 17 世纪前半期所发展,后者是 Leibniz 和 Newton 在 17 世纪后半期及 18 世纪初发展的。

微分几何出现在 18 世纪稍晚的时候,以欧拉的工作"*Recherches sur la curbure des surfaces*"(1760)(曲面曲率的研究)和 Monge 的工作"*Une application de l'analyse a la geomerie*"(1975)(分析在几何中的应用)为代表。在高斯的奠基性文章"*Disquisitiones generals circa suoerficies curves*"(弯曲曲面的一般研究)于 1827 年用拉丁文(在 Spivak 的书(1979)中可找到它的部分英译内容)出版之前,嵌入 R^3 中的曲面或是用一个方程 $W(x,y,z)=0$ 来描述,或是用一个变量由其他两个变量来表示。尽管欧拉已注意到曲面上一点的坐标可表示为两个独立变量的函数,但正是高斯,第一个系统使用这样的参数表示,从而引发出作为微分几何基础的"局部坐标长"的概念。

微分流形

与欧氏空间中特殊嵌入无关的 n 维流形的真实概念可追溯到 1854 年 Riemann 在 Göttingen 大学发表的一个演讲"*Uber die Hypothesen, welche der Geomerie zu Grunde liegen*"(关于作为几何学基础的假设)[可以在 Spivak 的书中找到英译文和注释(1979)],他在演讲中清楚地指出,n 维流形局部地类似于 n 维欧氏空间。Riemann 在他的工作中提到了无限维流形的存在,如函数空间,在今天扮演着重要的角色,因为它们在量子场论中作为构形空间而自然地出现。

用现代的语言来说,同模于拓扑空间 V(可以是无限维的,如 Fréchet 空间,Banach 空间或 Hilbert 空间)的微分流形是一个具备一族局部坐标长 $(U_i,\varphi_i)_{i\in I}$ 的拓扑空间 M,使得开子集 $U_i\subset M$ 全体覆盖 M,其中 $\phi_i:U_i\to V(i\in I)$ 是同胚,它们给出光滑转移映射 $\phi_i\cdot\phi_j^{-1}:\phi_j^{-1}(U_i\cap U_j)\to\phi_i(U_i\cup U_j)$。一个 n 维微分流形就是同模于 R^n 的微分流形。球面

$S^n:=\left\{x=(x_1,\cdots,x_2)\in R^n\,\middle|\,\sum x_i^2=1\right\}$ 是一个 $n-1$ 维微分流形。

R^n 中的简单可微曲线是一个一维流形,局部地由坐标 $x(t)=(x_1(t),\cdots,x_n(t))\in R^n$ 确定,其中 $t\to x_i(t)$ 是 C^k 阶的。这种曲线在点 $x(t_0)$ 处的切线就是过该点、方向由 $x'(t_0)$ 决定的直线;这可推广为同模于 V 的光滑流形 M 在点 $m\in M$ 的切空间 T_mM 的概念,它是一个与 V 同构的向量空间,由一切 $\gamma(t_0)=m$ 的 C^1 阶曲线 $\gamma(t)$ 在点 m 的切向量所张成。

为了使它更精确,我们需要可微映射的概念。给定两个微分流形 M 和 N,一个映射 $f:M\to N$ 在点 m 是可微的,如果对于 M 的每个包含 m 的坐标图 (U,ϕ) 和每个满足 $f(U)\subset V$ 的 N 的坐标图 (V,ψ),映射 $\psi\circ f\circ\phi^{-1}:\phi(U)\to\psi(V)$ 在点 $\phi(m)$ 是可微的。特别地,所有可微映射 $f:M\to R$ 形成了 M 上光滑实值函数的代数 $C^\infty(M,R)$。从一个区间 $[a,b]\subset R$ 到微分流形 M 的可微映射 $\gamma:[a,b]\to M$ 称为 M 上的"可微曲线"。如果可微映射 $f:M\to N$ 是可逆的,且其逆 $f^{-1}:N\to M$ 也是可微的,则称 f 为微分同胚。

一个函数 $f\in C^\infty(M,R)$ 沿一曲线 $\gamma:[a,b]\to M$ 在点 $\gamma(t_0)\in M(t_0\in[a,b])$ 的导数由下式

$$Xf:=\frac{\mathrm{d}}{\mathrm{d}t}_{|t=t_0}f\circ\gamma(t)$$

给出,而映射 $f\mapsto Xf$ 称为曲线 γ 在点 $\gamma(t_0)$ 的切向量。所有曲线 $\gamma:[a,b]\to M$ 在给定点 $m\in\gamma[a,b]$ 的切向量构成了一个向量空间 T_mM,称为 M 在点 m 的切空间。

对每点 $m\in M$ 指定一个切向量 $X\in T_mM$ 的一个(光滑)映射称为一个(光滑)向量场。它也可以看作对于任何 $m\in M$,由 $(\tilde{X}f)(m):=X(m)f$ 定义的 $C^\infty(M,R)$ 上的一种求导算子 $\tilde{X}:f\to Xf$,从而向量场的方括号可由算子方括号 $[\tilde{X},\tilde{Y}]=\tilde{X}\circ\tilde{Y}-\tilde{Y}\circ\tilde{X}$ 来定义。切向量的线性运算可在向量场上实施 $(X+Y)(m):=X(m)+Y(m)$,$(\lambda X)(m)=\lambda X(m)$,其中 $m\in M,X,Y\in T_mM,\lambda\in R$,因而 M 上的向量场构成了一个线性空间。

也可借助 M 上的局部单参数可微变换群来生成切向量,也即从 $[-\varepsilon,\varepsilon]\times U$ 到 U(其中 $\varepsilon>0$ 且 $U\subset M$ 是 M 的开集)的映射 $(t,m)\mapsto\phi_t(m)$,使得 $\phi_0=Id$,$\phi_{t+s}=\phi_t\circ\phi_s$($\forall s,t\in(-\varepsilon,\varepsilon)$ 和 $t+s\in(-\varepsilon,\varepsilon)$),且 $m\mapsto\phi(m)$ 是 U 到开子集 $\phi_t(U)$ 上的微分同胚。曲线 $\gamma(t)=\phi_t(m)$ 在 $t=0$ 处的切向量导出一个在点 $m=\gamma(t)$ 处的 M 的切向量。反之,当 M 为有限维时,根据常微分方程组的基本定理得出:对于 M 上的任何向量场 X,存在(在 M 上任一个点 $m\in M$ 的周围)一个局部单参数局部变换群 $\phi:(-\varepsilon,\varepsilon)\times U\to M$($U$ 是一个包含 m 的开子集),使它诱导出切向量 $X(m)\in T_mM$。

一个可微映射 $\phi:M\to N$ 诱导出一个映射 $\phi_*(m):T_mM\to T_{\phi(m)}N$,它定义为 $\phi_*Xf=X(f\circ\phi)$。流形 M 到流形 N 的一个"浸入"是一个可微映射 $\phi:M\to N$,使得在任何点 $m\in M$,$\phi_t(m)$ 是单射。若这样的映射还是同胚,则称为嵌入,此时称 $\phi(M)\subset N$ 是 N 的一个子流形。单位球面 S^n 是 R^{n+2} 的一个子流形。Whitney 证明了:任意一个光滑的 n 维实流形总可以嵌入到 R^{2n+1} 中。

若一个微分流形的坐标图取值在复向量空间中,且转移映射是全纯的,则称为复流形。若 $V=C^n$,则它是复 n 维的。复射影空间 CP^m,即 C^{n+1} 中所有过 0 的复直线的全体是一个 n 维紧复流形。类似于微分流形间可微映射的概念,我们也有复流形间全纯映射的概念。

微分流形 M 上切空间 T_mM 的自同态 J_m 的一个光滑族 $m\mapsto J_m$,若满足 $J_m^2=-Id$,

则给出了一个殆复流形。其原型是 C^n 上的殆复结构 J_m,它定义为 $J_m(\partial_{x_i})=\partial_{y_i}$,$J_m(\partial_{y_i})=-\partial_{x_1}$,其中 $z=(x_1+iy_1,\cdots,x_n+iy_n)\in C^n$。利用局部坐标图,这可以转换到一个复流形上。流形 M 上的一个殆复结构 J 称为复的,如果 M 是通过上述方式导出 J 的基础微分流形。

研究微分流形上的光滑函数能提供关于流形拓扑的信息。例如,一个紧流形上的光滑函数的性态,如它的临界点等,都被流形的拓扑性质所强烈限制。这导致了 Morse 临界点理论,它可推广到无限维流形;在其他一些结果中,引出了关于变分问题的极值曲线或闭极值曲线的某些结论。与其考虑流形上的特殊点,不如从函数空间的观点来研究其流形几何。这就导致了研究微分几何的一种代数方法。初始的概念是存在一个交换环(在非交换几何的框架下它可能是非交换代数),即流形上的光滑函数环,而流形本身被这环定义为其极大理想的空间。特别地,为了理解超流形(一种对超对称场论很重要的广义流形),这个观点被证明是很有效的。

我们可以进一步考虑流形的开子集上光滑函数的层,这个观点导致了层论,它提供了一种建立拓扑空间的局部与整体性质之间联系的统一方法。

度量性质

Riemann 关注于流形的度量性质,但把一个具备度量的流形的概念第一次清晰地公式化是由 Weyl 在其著作"*Die Idee der Riemannsche Fläche*"中给出的。微分流形 M 上的一个黎曼度量是 T_mM(对每一个点 $m\in M$)上的一个正定内积 g_m,它光滑地依赖于点 m。具备黎曼度量的流形称为黎曼流形。黎曼度量乘以一个光滑正函数的 Weyl 变换,产生一个新黎曼度量,它与原度量有相同的角度值,因而保持 M 上的"共形"结构不变。

Riemann 也建议考虑切空间上不是从内积诱导的度量;流形上以这种方式建立的度量首先是被 Finsler 进行系统的研究,所以被称为 Finsler 度量。黎曼流形 M 上的测地线相当于这样一条光滑曲线 $\lambda:[a,b\}\to M$,它使长度泛函

$$L(\gamma):=\frac{1}{2}\int_a^b\sqrt{g_{\gamma(t)}\left(\frac{\mathrm{d}\gamma}{\mathrm{d}t},\frac{\mathrm{d}\lambda}{\mathrm{d}t}\right)}\,\mathrm{d}t$$

极小化,因而测地线推广了实现充分接近的两点之间最短距离的曲线。

自然导入黎曼几何的 Euclid 公理,除平行性公理外,也都能满足。平行性公理被 Lobatchevsky 在 1829 年和 Bolyai 在 1832 年发展出一种(双曲)几何。非欧几何实际上在微分几何的发展中扮演了较重要的角色。Lobatchevsky 的工作鼓舞了 Riemann 及后来的 Klein。

放弃 T_mM 上双线性形式 g_m 的正定性假设,就导致了 Lorentz 流形,它是一个在切空间上装备了符号差为 $(1,n)$ 的双线性形式的 $n+1$ 维光滑流形。这些出现在广义相对论中,并且长度平方为负、正或零的切向量分别称为类时、类空和类光。

就像复向量空间可装备一个正定的 Hermite 数积,一个复流形 M 可以装备一个 Hermite 度量,即在每点 $m\in M$ 的 T_mM 上装备一个正定的 Hermite 内积 h_m,并且光滑地依赖于点 m。每一个 Hermite 度量的实部给出了一个黎曼度量。复射影空间 CP^n 自然地具备 Fubini-Study Hermite 度量。

变换群

度量性质可以从变换群的观点来理解。Poncelet 在他的著作"*Traité projectif des figures*"(1822)中已从射影几何的观点研究了经典欧氏几何,但是直到 Cayley(1858)时期,度量性质才被解释为在任何"射影"变换下稳定不变的性质,这种变换保持"虚圆点"(复平面虚轴上的无穷远点)不变。S. Lie 进一步研究了变换群,导致了李群的现代概念,即赋予群结构的光滑流形,使得群运算是光滑的。

李群 G 上的向量场 $\boldsymbol{X}$ 被称为左(或右)不变的,如果对任意的 $g\in G$,X 在左移动 L_g:$h\to gh$(或右移动 R_g:$h\to hg$)下不变,也即 $\forall (g,h)\in G^2$,有 $(L_g)_*\boldsymbol{X}(h)=\boldsymbol{X}(gh)$(或者 $(R_g)_*\boldsymbol{X}(h)=\boldsymbol{X}(hg)$)。所有左不变向量场的集合,装备了求和、数乘及向量场的方括号运算后,就构成了一个代数,称为 G 的李代数。

所有实(或复)可逆 $n\times n$ 矩阵的群 $Gl_n(R)$(或 $Gl_n(C)$)是一个具有李代数 $gl_n(R)$(或 $gl_n(C)$)的李群,这里 $gl_n(R)$(或 $gl_n(C)$)是所有实(或复)$n\times n$ 矩阵连同方括号运算为 $[\boldsymbol{A},\boldsymbol{B}]=\boldsymbol{AB}-\boldsymbol{BA}$ 的代数。

正交(或酉)群 $O_n(R):=\{\boldsymbol{A}\in Gl_n(R),\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}=1\}$ 是一个紧李群,其中 $\boldsymbol{A}^{\mathrm{T}}$ 表示 $\boldsymbol{A}$ 的转置矩阵(或 $U_n(C):=\{\boldsymbol{A}\in Gl_n(C),\boldsymbol{A}^*\boldsymbol{A}=1\}$,其中 $\boldsymbol{A}^*=\bar{\boldsymbol{A}}^{\mathrm{T}}$),它的李代数为 $o_n(R):=\{\boldsymbol{A}\in Gl_n(R),\boldsymbol{A}^{\mathrm{T}}=-\boldsymbol{A}\}$(或 $u_n(C):=\{\boldsymbol{A}\in Gl_n(C),\boldsymbol{A}^*=-\boldsymbol{A}\}$)。

有限维李群 G 上的左不变向量场 $\boldsymbol{X}$(或等价的,G 的李代数的一个元素 $\boldsymbol{X}$)生成一个整体单参数变换群 $\phi_{\boldsymbol{X}}(t)$,$t\in R$。由 $\exp(\boldsymbol{X}):=\phi_{\boldsymbol{X}}(1)$ 定义的从 G 的李代数到 G 的映射称为指数映射。$Gl_n(R)$(或 $Gl_n(C)$)的指数映射由级数 $\exp(\boldsymbol{A})=\sum_{i=0}^{\infty}\boldsymbol{A}^i/i!$ 给出。

作为物理系统的对称群,李群在物理学中扮演了重要的角色,特别是在量子力学和 Yang-Mills 理论中。无限维李群是作为对称群出现的,例如广义相对论中流形上的微分同胚群,Yang-Mills 理论中的规范变换群,弦理论中曲面上度量的 Weyl 变换群。"物理应该与它的如何描述无关"这一原则就转变成在对称群(可能是无限维群)作用下的不变性。当这样的不变性对物理理论的经典作用成立而对量子水准却"破缺"时,反常情况就出现了。

Klein 在他的 Erlangen 纲领(1872)中,把变换群的概念放到了最显著的地位,他引进了一种新颖的思想:人们应该考虑具有某些性质的空间,例如在给定变换群下不变的对象的集合。因而可以根据一个特殊问题与什么群有关,而把几何结果进行分类。例如,对于射影几何的射影线性群,对于黎曼几何的正交群,或对于"辛"几何的辛群。

纤维丛

变换群引出了在 Yang-Mills 理论中有重要地位的主纤维丛。纤维丛记号最早出现在 20 世纪 30 年代关于流形的拓扑和几何所提出的问题中。1950 年左右,Steenrod 清晰地给出了纤维丛的公式化定义。

一个具有典型纤维流形 F 的光滑纤维丛是一个三元组(E,π,B),其中 E 和 B 是光滑流形,分别称为全空间和底空间,$\pi:E\to B$ 是光滑满映射,称为丛的投影,使得 $b\in B$ 的原像 $\pi^{-1}(b)$ 与 F 同构,称为 b 的纤维,并且任何基点 b 都有一个领域 $U\subset B$,使得原像 $\pi^{-1}(U)$ 与 $U\times F$ 微分同胚,这里的微分同胚与底空间的投影映射可交换。E 的光滑截面

是映射$\sigma:B\to E$,使得$\pi\circ\sigma=I_B$。

当F是一个向量空间,并且给定覆盖B的开子集$U_i\subset B(i\in I)$和相应的坐标图$(U_i,\phi_i)_{i\in I}$时,局部微分同胚$\tau_i:\pi^{-1}(U_i)\approx\phi_i(U_i)\times F$给出转移映射$\tau_i\circ\tau_j^{-1}:\phi_j(U_i\cap U_j)\times F\to\phi_i(U_i\cap U_j)\times F$,它在纤维上是线性的,这时该丛称为"向量丛"。同模于向量空间V的微分流形M的切丛$TM=\bigcup_{m\in M}T_mM$是一个具有典型纤维V的向量丛,其转移映射$\tau_{ij}=(\phi_i\circ\phi_j^{-1},d(\phi_i\circ\phi_j^{-1}))$可用流形$M$上的转移映射的微分来表达。切丛的对偶丛——余切丛,以及切丛与余切丛的张量积也都是向量丛,它们分别具有典型纤维V^*(V的对偶空间)及V与V^*的张量积。前面定义的向量场是切丛的截面,M上的1形式是余切丛的截面,反变张量场(或协变张量场)是切丛(或余切丛)的张量积的截面。一个可微映射$\phi:M\to N$把N上的协变p张量场T通过ϕ拉回成M上的协变p张量场,它给定如下:

$$(\phi^*T)(X_1,\cdots,X_p):=T(\phi_*X_1,\cdots,\phi_*X_p),$$

其中$X_1,\cdots,X_p$是M上的任意向量场。

M上一个光滑函数f的微分给出M上的一个1形式$\mathrm{d}f$。更一般地,p次外形式ω是反对称的光滑协变p张量,从而$\omega(X_{\sigma(1)},\cdots,X_{\sigma(p)})=\varepsilon(\sigma)\omega(X_1,\cdots,X_P)$,其中$X_1,\cdots,X_p$是$M$上的任意向量场,$\sigma\in\Sigma_p$是具有符号$\varepsilon(\sigma)$的置换。

黎曼度量是协变(对称)2张量,流形M上所有黎曼度量的空间是一个无限维流形,它作为构形空间出现在弦理论和广义相对论中。

主丛是一个以李群G为典型纤维的纤维丛(P,π,B),其中G通过右作用$(p,g)\in P\times G\mapsto pg=R_g(p)\in P$自由而正常地作用在全空间$P$上,使得局部微分同胚$\pi^{-1}(U)\approx U\times G$是$G$等变的。给定一个主纤维丛$(P,\pi,B)$,它以有限维李群$G$作为结构群。$G$在$P$上的作用诱导了一个同态:对$G$的李代数的任一元素$X$,指定$P$上的一个向量场$X^*$,称为由$X$生成的"基本向量场"。它在点$p\in P$定义为

$$X^*(p):=\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0}R_{\exp(tX)}(p),$$

其中exp是G上的指数映照。

给定G在向量空间V上的一个作用,就可以通过以G为典型纤维的主丛,构造一个以V为典型纤维的配丛。主丛在规范理论中是本质的;$U(1)$主丛出现在电磁学中,而非交换结构群出现在Yang-Mills理论中。在那里,场就是主丛上的联络,规范变换在(不可约)联络上的作用导出了模空间上的一个无限维主丛,它的结构群由规范变换给出。无限维的丛也出现在其他的场论中,如弦理论,其中模空间对应于黎曼面上不等价的复结构,它的无限维结构群可由度量的Weyl变换和曲面的微分同胚构造出来。

联络

在一个流形上,不存在典范的方法将不同点处的切空间等同起来。为了微分向量场,需要这种等同,而在黎曼流形上可以通过向量场的"平行移动"来获得这种等同。黎曼流形上协变微分理论的基本观念在19世纪末由Ricci提出,更完善的形式出现在1901年与Levi-Civita合作的书"*Methodes de calcul differentiel absolu et leurs applications*"中;在黎曼流形上,以典范的方法定义向量的平行移动是可能的,从而利用后来所谓的Levi-Civita联络可对向量场进行协变微分。

更一般地,流形 M 的向量丛 E 上的一个(线性)联络(或者等价的一个协变求导)提供了将向量丛中不同点处的纤维等同起来的一种方式;这是将 E 中的截面变为 M 上 E 值 1 形式的一个映射 ∇,它满足 Leibniz 法则 $\nabla(f\sigma)=\mathrm{d}f\sigma+f\nabla\sigma$,其中 f 是 M 上的任意光滑函数。当 E 是 M 的切丛时,流形上具有协变常速 $\nabla\dot{\gamma}(t)=0$ 的曲线 γ 给出了测地线。给定初始速度 $\dot{\gamma}(0)=X\in T_mM$ 并设 X 具有足够小的范数,那么 $\gamma_X(1)$ 定义了相应测地线上的一点,从而映射 $\exp:X\mapsto\gamma_X(1)$ 将 T_mM 的原点 0 的一个邻域与 $m\in M$ 的一个邻域微分同胚,它称为 ∇ 的"指数映射"。

联络在主丛上的推广,是 Ehresmann 在 Cartan 工作的基础上发展起来的。以 G 为结构群的主丛 (P,π,B) 上的一个联络,是切空间 T_pP 的一个光滑等变(在群 G 的作用下)分解 $T_pP=H_pP\oplus V_pP$,它将每点 p 处的切空间分解为水平空间 H_pP 和垂直空间 $V_pP=\mathrm{Ker}\ \mathrm{d}\pi_p$。主丛上的联络可以导出配丛上的线性联络。

P 上的联络给出 P 上的一个 1 形式 ω,它取值于结构群 G 的李代数,称为联络 1 形式,其定义如下:对于任意 $X\in T_pP$,$\omega(X)$ 是 G 的李代数里惟一的元 U,使得相应的基本向量场 $U^*(p)$ 在 p 点与 X 的垂直分量重和。特别地,对于 G 的李代数中的任何 U,有 $\omega(U^*)=U$。

联络组成的空间是一个无限维空间,在 Yang-Mills 理论中作为构形空间而出现,并且也在 Seiberg-Witten 理论中发挥作用。

几何微分算子

在黎曼流形上,可通过联络来定义一系列微分算子,其中包括二阶 Laplace 算子。特别地,作用在光滑函数上的 Laplace-Beltrami 算子 $f\mapsto-\mathrm{tr}(\nabla^{T^*M}\mathrm{d}f)$ 推广了欧氏空间中通常的 Laplace 算子,其中 ∇^{T^*M} 是余切丛上由 M 的 Levi-Civita 联络所诱导的联络。这也可以推广为作用在向量丛 E 的光滑截面上的二阶算子 $\Delta^E:=-\mathrm{tr}(\nabla^{T^*M\otimes E}\nabla^E)$,其中 ∇^E 是 E 上的联络,$\nabla^{T^*M\otimes E}$ 是 $T^*M\otimes E$ 上由 ∇^E 和 Levi-Civita 联络诱导的联络。

自旋型黎曼流形上的 Dirac 算子是一阶微分算子,在不计零阶项时,它的平方与 Laplace-Beltrami 算子一致。对 Dirac 算子的最好理解是追溯 Dirac 算子的原始想法。系数为常矩阵的一阶微分算子 $\sum_{i=1}^{n}\gamma_i(\partial/\partial x_i)$ 的平方是 R^n 中的 Laplace 算子 $-\sum_{i=1}^{n}\partial^2/\partial x_i^2$,当且仅当它的系数满足 Clifford 关系

$$\gamma_i^2=-1,\forall\ i=1,\cdots,n$$

$$\gamma_i\gamma_j+\gamma_j\gamma_i=0,\forall\ i\neq j$$

所得的 Clifford 代数经过复化之后,在偶数维 $n=2k$ 时同构于空间 $\mathrm{End}(S_n)$(奇数维 $n=2k+1$ 时为 $\mathrm{End}(S_n)\oplus\mathrm{End}(S_n)$),这里 $\mathrm{End}(S_n)$ 表示复 n 维旋量空间 $S_n=C^{2k}$ 的自同态空间。若我们从切丛 TM 上由 M 的黎曼度量所诱导的度量出发,取代 R^n 上的典则度量,并且假设相应的旋量空间能组成 M 上的一个"旋量丛",那么 M 称为一个自旋流形。自旋黎曼流形 M 上的 Dirac 算子是作用在旋量上的一阶微分算子 $D_g=\sum\gamma\nabla\ \mathrm{e}_i$,其中 ∇ 是旋量(旋量丛 S 的截面)上的联络,它由 Levi-Civita 联络诱导,$\mathrm{e}_1,\cdots,\mathrm{e}_n$ 是切丛 TM 上的一个幺正标架。这是更广泛的挠 Dirac 算子 $D_g{}^W$ 的特殊情况,$D_g{}^W$ 定义在具有联络 $\nabla^{S\otimes W}$ 的挠旋量丛 $S\otimes W$ 上,其中 $\nabla^{S\otimes W}$ 是联络 ∇ 和辅助向量丛 W 上的联络 ∇^W 的联合。

挠 Dirac 算子的平方$(D_g{}^W)^2$与 Laplacian $\Delta^{S\otimes W}$有关，后者是利用挠联络通过 Lichnerowicz 公式建立起来的。Lichnerowicz 公式对于用基础几何数据估计 Dirac 算子的谱很有用。

当 M 上没有自旋结构时，仍能希望有 Spin^c 结构及与这一结构相容的联络导出的 Dirac D^C 算子。特别地，每个紧致定向的 4 流形可以配备一个 Spin^c 结构，还可通过两个偏微分方程的解建立微分流形上的 Seiberg-Witten 不变量，其中一个微分方程是 Dirac 方程 $D^C\Phi=0$，这里的联络与 Spin^c 结构相容；另一个是包含曲率的非线性方程。

曲率

现今用联络来理解的“曲率”概念（联络 ∇ 的曲率定义为 $\Omega=\nabla^2$）在历史上是先于联络出现的。曲率概念的现代模式可追溯到高斯。利用曲面的球面表示——高斯映射 ν，将定向曲面 $\Sigma\subset R^3$ 上的一点 m 映为单位外法向量 ν_m，高斯定义了在点 $m\in U\subset\Sigma$ 的此后被称为高斯曲率的 K_m，它是当 U 的面积趋向于零时比值 $\mathrm{area}(\nu(U))/\mathrm{area}(U)$ 的极限。高斯曲率表达了寻找从点 m 附近的曲面片到标准平面区域的等距变换的障碍程度。高斯美妙定理指出：R^3 中光滑曲面的高斯曲率可由曲面的度量来确定，因而两张等距曲面的高斯曲率是一致的。

在黎曼流形 (M,g) 上，从联络的曲率 Ω 可以构造黎曼曲率张量，这是一个 4 张量，在局部坐标系下可表示为

$$R_{ijkl}:=g\left(\Omega\left(\frac{\partial}{\partial_i},\frac{\partial}{\partial_j}\right)\frac{\partial}{\partial_k},\frac{\partial}{\partial_l}\right)。$$

进而取部分迹可得到 Ricci 曲率，它由 2 张量 $Ric_{ij}=\sum R_{ikjk}$ 给出[①]。它再取迹可得数量曲率 $R=\sum Ric_{ii}$[②]。点 m 处由单位向量 U,V 张成的二维平面方向的截面曲率等于 $K(U,V)=g(\Omega(U,V)V,U)$。若对所有线性无关的向量 U 和 V，$K(U,V)/\|U\wedge V\|^2$ 均为常数 K，则流形具有常截面曲率。一个具有常截面曲率的黎曼流形称为球型的、平坦的或双曲型的，如果分别有 $K>0$、$K=0$ 或 $K<0$。对称空间是一类重要的黎曼流形，它的发现归功于 Cartan，它们包括了球面、欧氏空间、双曲空间和紧致李群。如果连通黎曼流形 M 上的每个点 m 都存在等距 σ_m，使得 $\sigma_m(m)=m$ 且切空间上的切映射 $T_m\sigma_m$ 等于 $-Id$（从而使得过 m 的测地线反向），那么 M 称为对称的。具备 Fubini-Study 度量的 CP^n 是对称空间，它的等距是 C^{n+1} 中关于直线的反射。紧致对称空间具有非负截面曲率 K。

对曲率的限制可以得到流形的拓扑结论。球面是惟一的具有正常数截面曲率的单连通流形；若维数大于 1 的单连通完备黎曼流形具有非正截面曲率，则它同胚于欧氏空间。

Ricci 曲率张量与度量张量成比例的流形称为爱因斯坦流形。自爱因斯坦以来，曲率就是广义相对论的基础，其中重力用曲率来解释。譬如，真空爱因斯坦方程为 $Ric_g=(1/2)R_gg$，其中 Ric_g 是度量 g 的 Ricci 曲率，R_g 是数量曲率。另外，Kaluza-Klein 超重力是一个统一理论，它的模型是四维 Minkowski 空间和正数量曲率的爱因斯坦流形的直积。

与广义相对论中爱因斯坦方程有关的 Ricci 流 $\mathrm{d}g(t)/\mathrm{d}t=-2Ric_{g(t)}$，不久前才刚刚被引入数学文献。以 Ricci 流为本质性方法，要得到三维闭流形的分类是大有希望的。

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①，②　在幺正标架下——译者注。

上同调

微分流形 M 上函数的微分 $f\to \mathrm{d}f$ 可以推广为微分形式的外微分 $\alpha\to \mathrm{d}\alpha$。如果一个形式是 d 的核的元素,则该形式称为闭形式,如果它是 d 的值域的元素,则称为恰当形式。由于 $\mathrm{d}^2=0$,因此恰当形式一定是闭形式。

Cartan 结构方程 $\mathrm{d}\omega=\frac{1}{2}[\omega,\omega]+\Omega$ 把主丛上联络 1 形式 ω 的外微分和其上的曲率 Ω 联系起来。Ω 是由对 ω 的协变外微分 $D\omega:=\mathrm{d}\omega\circ h$ 给出,其中 $h:T_pp\to H_pp$ 是到水平空间上的投影映射。

在一个复流形上,形式分解成 (p,q) 形式之和,(p,q) 形式包含 p 全纯分量和 q 反全纯分量。因而外微分算子 d 也分成解全纯和反全纯两个部分,即 $d=\partial+\bar{\partial}$,并有 $\partial^2=\bar{\partial}^2=0$。

几何条件通常是用某些微分形式的闭性条件给出的,例如一个"辛流形"就是具有一个闭的非退化 2 形式的微分流形 M,这个 2 形式称为"辛形式"。在具有殆复结构 J 的流形上,J 全纯曲线理论在建立辛流形的不变量方面被证明是很有用的。一个 Kähler 流形是具有 Hermite 度量 h 的复流形,使得 h 的虚部 $\mathrm{Im}h$ 是一个闭的 $(1,1)$ 形式。复射影空间 CP^n 是 Kähler 流形。

外微分算子 d 给出的 de Rham 上同调群是 $\ker d/\mathrm{Im}\, d$,而 de Rham 定理建立了 de Rham 上同调群和流形的实奇异上同调群之间的一个同构。陈(示性)类是纤维丛上的拓扑不变量,并且在指标理论中起着关键性的作用。陈-Weil 理论建立了这些 de Rham 上同调类的表示,其中用到了形如 $\mathrm{tr}(f(\nabla^2))$ 的式中的联络 ∇,这里 f 是某个解析函数。

当流形是黎曼流形时,作用在函数上的 Laplace-Beltrami 算子可通过两种不同方式推广到微分形式上。一种是作用在形式(即 $\wedge T^*M$ 的截面)上的 Bochner-Laplacian 算子 $\Delta^{\wedge T^*M}$,这里余切丛 T^*M 具有由 Levi-Civita 联络诱导的联络。另一种是作用在形式上的 Laplace-Beltrami 算子 $(\mathrm{d}+\mathrm{d}^*)^2=\mathrm{d}^*\mathrm{d}+\mathrm{d}$,其中 d^* 是 d 的伴随算子。这些算子通过 Weizenböck 公式联系起来;在 1 形式的特殊情形下,Weizenöck 公式指出,这两个算子之差可用 Ricci 曲率来测量。

当流形是紧致时,Hodge 定理表明,de Rham 上同调群同构于调和(即被 Laplace-Beltrami 算子所零化)微分形式的空间。因此,调和 k 形式集合的维数等于第 k 个 Betti 数,由此可定义流形 M 的欧拉示性数 $\chi(M)$,即取 Betti 数的代数和。Hodge 理论在镜对称性中起着重要的作用,在几何上,镜对称性提供了不同流形之间的一种对偶性;在物理上,通过相关函数,镜对称性提供了不同场论之间的一种对偶性。Calabi-Yau 流形是 Ricci 平坦的 Kähler 流形,在对偶性的产生背景中它们被广泛地研究。

指标理论

尽管高斯曲率是局部问题的解,但它对曲面的整体拓扑有很强的影响。Gauss-Bonnet 公式(1850)把闭曲面 M 上的欧拉示性数和高斯曲率联系起来,即

$$\chi(M)=\frac{1}{2\pi}\int_M K_m\,\mathrm{d}A_m$$

其中 $\mathrm{d}A_m$ 是 M 上的面积元。这是关于曲率和整体性质的第一个结果,并且可看作是指

标理论的出发点之一。Chern-Gauss-Bonner 定理(1944)把 Gauss-Bonner 定理推广到偶维数的闭流形上,并可以看作下述 Atiyah-Singer 指标定理(1963)的特例:

$$\mathrm{ind}(D_g^W) = \int_M \widetilde{A}(\Omega_g)\mathrm{e}^{-\mathrm{tr}(\Omega^W)}$$

其中 g 表示一自旋流形 M 上的黎曼度量,D_g^W 是作用在某个挠丛 $S\otimes W$ 上的 Dirac 算子,这里 S 是 M 上的旋量丛,W 是 M 上的辅助向量丛。$\mathrm{ind}(D_g^W)$ 是 Dirac 算子的"指标",Ω_g 和 Ω^W 分别表示 Levi-Civita 联络和 W 上的联络,$\widetilde{A}(\Omega_g)$ 是一特殊的 Chern 形式,称为 $\widetilde{\mathrm{A}}$ 亏格。在出自经典作用量的泛函型量子化规范理论中,指标定理对计算其反常是很有用的。

给定一个偶维数的自旋闭流形 (M,g) 和 M 上的一个 Hermite 向量丛 W。由相关的 Dirac 算子 D_g^W 的指标可得到所谓的 Atiyah 映射 $K^0(M)\to Z$,它定义为 $W\to\mathrm{ind}(D_g^W)$,其中 $K^0(M)$ 是 M 上光滑向量丛的稳定同伦类的形式差群。这是指标理论中非交换几何方法的出发点,其中由于 $K^0(M)\approx K_0(C^\infty(M))$(在矩阵空间 $gl_n(C^\infty(M))$ 的归纳极限下,它由幂等的光滑同伦类的形式差所组成),以隐蔽形式出现的流形上的光滑函数空间被推广到任何非交换光滑代数中。

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导论:电磁学

引言

电磁学现代理论的基础是麦克斯韦方程组,

$$\mathrm{div}\boldsymbol{E} = \frac{\rho}{\varepsilon_0} \qquad [1]$$

$$\mathrm{div}\boldsymbol{B} = 0 \qquad [2]$$

$$\mathrm{curl}\boldsymbol{B} - \frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} = \mu_0 \boldsymbol{J} \qquad [3]$$

$$\mathrm{curl}\boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0 \qquad [4]$$

公式的左边是电场 $\boldsymbol{E}$ 和磁场 $\boldsymbol{B}$,它们是位置和时间的矢值函数,公式的右边是源,电荷密度 ρ 和电流密度 $\boldsymbol{J}$,前者是位置和时间的标量函数。源项表述成电荷的分布和速度,而方程组连同在无穷远处的边界条件确定了它们所激发的场。根据这些方程,可导出静电学和静磁学熟知的各种预言,以及场和电荷的动力学行为,特别是电磁波——光波的激发和传播。

麦克斯韦没有认识到这些方程紧凑的矢量表达形式,更不用说它们在狭义相对论中的张量形式。值得注意的是虽然在方程组的命名上他的贡献普遍被承认,但是很少见到引证"麦克斯韦理论"。这是大家认同的说法。麦克斯韦在他电磁学的早期研究中依据精心制作的力学模型工作,他把它看成类比物,而不是根本的物理实在的文字描述。在他的后期工作中,力学模型,特别是传播光波的"传光以太"的力学性质作为电磁理论的基础更为文字化地提出来了。在现代理论中,方程组幸存下来,但麦克斯韦、法拉第,以及其他人为之奋斗的力学模型只在如"力线"、"磁通量"等陈旧的术语残存中还存在。传光以太在狭义相对论出现之后就消散了。

麦克斯韦的遗产不是他的理论,而是他的方程组:一个和谐一致的偏微分方程组体系,它描述了电场和磁场与运动电荷间已知相互作用的整个领域。通过第一次揭示电场和磁场之间充分的对偶性,来统一处理电学和磁学。这组方程证实了几乎不可想像的各种各样的物理过程,从光通过星系磁场的行为而越过宇宙学距离的传播,电机和实验室实验的日常应用,一直到个别电子间交换光子。

麦克斯韦方程组的过去以许多人为的蜿蜒曲折旋绕着。麦克斯韦本人在他 1865 年论文"电磁场的动力理论"中对第一方程中的 ρ 以不同符号,写下方程组的不协调形式。而协调的形式迟至他的著作《电磁学通论》(1873)才出现,参见 Chalmers(1975)。

在本文中,我们将不按照历史的脉胳来谈方程组。上面某些评述中提到有关进展的复杂故事可在 Chalmers(1975),Siegel(1985)和 Roche(1998)的论文中找到。我们也将不按照许多教科书通过研究基本电磁现象建立充分的动力方程组这样一条传统的适宜于教学法的路线。替代之,我们将沿着这样一条路径到达麦克斯韦方程组,认识它

最关键的特征,即洛伦兹变换下的不变性,得出麦克斯韦方程组。当然,麦克斯韦对此一无所知。

我们将从有关电荷在电场和磁场中行为的基本事实概要出发,然后从不同运动参考系考察这一行为来建立充分的动力学构架。当然,自从麦克斯韦方程组与伽利略相对性不和谐以来,在时空的经典概念的构架内一致地这样做是不可能的。但是理解某些方程组的关键特征至少是可能的,特别是在麦克斯韦方程组第三方程中需要包含 $\boldsymbol{E}$ 的时间导数项,即所谓"位移电流"。

我们将从经典动力学中相对性所起作用的某些评论开始。

牛顿动力学中的相对性

牛顿定律在所有的惯性系中都成立。经典力学的形式体系在伽利略变换下是不变的,不可能通过观察粒子以及其他物体的动力学行为识别一个参考系是静止的还是在做匀速运动。因此在经典力学世界里:

相对性原理　不存在静止的绝对标准;只有相对运动是可观察的。

伽利略在他的《关于两大世界体系的对话》中通过辩论说明这一原理,如同在甲板下的船舱中观察到的那样,在平静海面上船的匀速行驶不影响鱼、蝴蝶和其他运动物体的行为。

相对性理论将这一原理作为基础,正如关于空间和时间本性的表述等同于关于牛顿运动方程特性的表述。但是如果给予其这种普遍意义,那么就必须适用于全部物理学,而不只是适用于牛顿动力学。最初这似乎不成问题,很难想像它在这种基本水平上成立,但不适用于更复杂的物理相互作用。尽管如此,当我们尝试将它扩展到电磁学时,由于伽利略不变性与麦克斯韦方程组相抵触,深度的问题还是显露出来。

对于含有慢速运动电荷以及慢变化电场和磁场的系统,一切都显得直截了当。它们看来像是被不同匀速运动参考系之间变换的不变性定律所支配。可以想像,伽利略船的现代方案也可以携带若干磁体、电池和半导体以及其他电性元件。萨尔维阿蒂对于相对性的论证似乎是强有力的。

当我们考虑迅变场,特别是当我们考虑光的传播时,问题就出现了。爱因斯坦(1905)指出,"麦克斯韦电动力学……,当应用到运动物体时导致一些不对称性,而这种不对称性似乎不是现象所固有的。"主要的困难是麦克斯韦方程组给光和其他电磁波一个确定的速度,在真空中它以相同的速度沿各方向传播,与源的运动无关,这一事实与伽利略不变性不相容,光在一个参考系中以速率 c 传播,在向着光源以速率 u 运动的参考系中必定具有速率 $c+u$。因此,对于光以任意速率传播必定是可能的,光在一个光源静止的参考系中以速率 c 传播,在运动参考系中应有某种其他速率,所以伽利略不变性意味着光速依赖于源的运动。

这一抵触的完满解决只能在狭义相对论中完成。值得注意的是,麦克斯韦方程组严格保留它的经典形式,但是做相对运动的参考系的空时坐标之间的变换却并不如此。当与光速相比较,所包含的速度不是无关紧要时,这种差别才显示出来,只要可忽略 u^2/c^2 级的项,麦克斯韦方程组与伽利略相对性原理就是协调的。

电荷、场和洛伦兹力定律

电磁理论现代形式中的基本对象是

- 荷电粒子
- 依赖于位置和时间的电场矢量 $\boldsymbol{E}$ 和磁场矢量 $\boldsymbol{B}$

粒子的电荷 e 可正可负,是类似于引力质量的固有量。它确定电场和磁场中粒子相互作用的强度,正如粒子的质量确定了引力场中粒子相互作用的强度。

这一相互作用有两方面。首先,电场和磁场对荷电粒子施加一依赖于电荷值、粒子速度及粒子所在处的 $\boldsymbol{E}$ 和 $\boldsymbol{B}$ 值的作用力。这个力由洛伦兹力定律给出,

$$\boldsymbol{f} = e(\boldsymbol{E} + \boldsymbol{u} \wedge \boldsymbol{B}) \qquad [5]$$

式中,e 是电荷,$\boldsymbol{u}$ 是速度。它类似于引力场 $\boldsymbol{g}$ 中作用于质量为 m 粒子的引力,

$$\boldsymbol{f} = m\boldsymbol{g} \qquad [6]$$

原则上借助于测定作用在具有已知速度的标准电荷上的作用力,通过力学定律,观察者可测量电场和磁场。

其次,运动电荷激发电场和磁场。但我们将不详细研究运动电荷激发场的方法,而只是陈述下列基本原理:

电磁基本原理 1 场线性依赖于电荷。

这意味着如果我们叠加两个电荷分布,则总的 $\boldsymbol{E}$ 场和 $\boldsymbol{B}$ 场是这两个分布分别激发的各自的场的和。

电磁基本原理 2 一个固定不动的点电荷 e 激发电场而不激发磁场,电场由下式给出,

$$\boldsymbol{E} = \frac{ke\boldsymbol{r}}{r^3} \qquad [7]$$

式中,$\boldsymbol{r}$ 是起于电荷的位置矢量,$r = |\boldsymbol{r}|$,k 是类似于引力恒量的正常量。

联合[7]和[5],我们得到两个固定不动电荷之间的静电力平方反比定律

$$\frac{kee'}{r^2} \qquad [8]$$

与重力不同,当电荷取相同符号时,是推斥力。

电磁基本原理 3 以速度 $\boldsymbol{v}$ 运动的点电荷激发磁场,

$$\boldsymbol{B} = \frac{k'e\boldsymbol{v} \wedge \boldsymbol{r}}{r^3} \qquad [9]$$

式中,k' 是第二个正常量。

此式是根据测定电路中流动电流所激发的磁场外推得来的。

电磁基本原理 2 和 3 中的常量 k 和 k' 确定了电磁相互作用的强度,它们通常表示为

$$k = \frac{1}{4\pi\epsilon_0}, \quad k' = \frac{\mu_0}{4\pi} \qquad [10]$$

电荷 e 用库[仑]量度,$|\boldsymbol{B}|$ 用特[斯拉]量度,$|\boldsymbol{E}|$ 用伏[特]每米量度,并用了 SI 单位制的其他量,

$$\epsilon_0 = 8.9 \times 10^{-12}, \mu_0 = 1.3 \times 10^{-6} \qquad [11]$$

电子的电荷是 -1.6×10^{-19}C,而通过电炉的电流是 $5 \sim 10\text{C} \cdot \text{s}^{-1}$。地球的磁场大约是 4×10^{-5}T;一根磁棒的磁场大约有 1T;牛律 Clarendon 实验室三楼大约有 50T 的磁场;

而中子星表面磁场大约是 10^8 T。

虽然我们在日常生活中更熟悉重力,但它比静电力弱得多,两个质子之间的静电推斥力比它们之间的引力吸引大 1.2×10^{36} 倍(在任何间隔上,两种力都遵从平方反比律)。

我们的目标是从电磁基本原理 1～3,用微分方程来置换[7]和[9],获得麦克斯韦方程组,而这些偏微分方程把场的强度与电荷连续分布的电荷密度 ρ 和电流密度 $\boldsymbol{J}$ 联系起来,这些密度定义为极限

$$\rho=\lim_{V\to0}\left(\frac{\Sigma e}{V}\right),\quad \boldsymbol{J}=\lim_{V\to0}\left(\frac{\Sigma e\,\boldsymbol{v}}{V}\right) \tag{12}$$

式中,V 是包含该点的小体积,e 是体积内的一个电荷,$\boldsymbol{v}$ 是它的速度,求和遍及 V 内的众多电荷,极限是取体积收缩(即便关于极限过程的精确处理我们没有太多的忧虑)。

固定不动的电荷分布

我们着眼于固定不动电荷分布的电场,开展把基本原理转换成偏微分方程的作业,其中采用高斯定理重新陈述平方反比定律来完成连续极限的通道。

高斯定理把电场沿闭合曲面的积分与它所包围的总电荷联系起来,对于一个点电荷,电场由电磁基本原理 2 给出:

$$\boldsymbol{E}=\frac{e\boldsymbol{r}}{4\pi\epsilon_0 r^3}$$

由于 $\mathrm{div}\boldsymbol{r}=3$ 和 $\mathrm{grad}r=\boldsymbol{r}/r$,我们有

$$\mathrm{div}\boldsymbol{E}=\mathrm{div}\left(\frac{e\boldsymbol{r}}{4\pi\epsilon_0 r^3}\right)=\frac{e}{4\pi\epsilon_0}\left(\frac{3}{r^3}-\frac{3\boldsymbol{r}\cdot\boldsymbol{r}}{r^5}\right)=0$$

除 $r=0$ 外,处处成立。所以用散度定理,对于包围不含有电荷的任意体积 V 的闭合曲面 ∂V 有

$$\int_{\partial V}\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}=0 \tag{13}$$

如果体积含有电荷,怎么办?考虑中心在电荷处半径为 R 的球面 S_R 包围的区域,S_R 有单位外法向矢量 $\boldsymbol{r}/r$,则

$$\int_{S_R}\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}=\frac{e}{4\pi\epsilon_0 R^2}\int_{S_R}\mathrm{d}S=\frac{e}{\epsilon_0}$$

特别是公式左边的面积分之值与 R 无关。

现在考虑闭合曲面 S 包围的任意有限体积,如果电荷不在体积内,则由[13],$\boldsymbol{E}$ 遍及 S 的积分为零。如果是这样,则可应用[13]到 S 和小球面 S_R 之间的体积 V,导致

$$\int_S\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}-\int_{S_R}\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}=\int_{\partial V}\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}=0$$

并且导致 $\boldsymbol{E}$ 遍及 S 和 S_R 的积分相同,因此

$$\int_S\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}=\begin{cases}e/\epsilon_0 & \text{如果电荷在被 } S \text{ 包围的体积内}\\ 0 & \text{其他情形}\end{cases}$$

当我们遍及电荷分布求和,公式左边的积分选择 S 内的总电荷,于是我们有高斯定理。

高斯定理 对于包围体积 V 的任意闭合曲面∂V,

$$\int_{\partial V}\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}=Q/\epsilon_0$$

式中,$\boldsymbol{E}$ 是总电场,Q 是 V 内的总电荷。

现在我们可以研究连续极限。假定 $\boldsymbol{E}$ 被具有密度 ρ(单位体积内的电荷)的电荷分布所激发,则由高斯定理,对任意体积 V 有

$$\int_{\partial V}\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}=\frac{1}{\varepsilon_0}\int_V\rho\mathrm{d}V$$

但是另一方面由散度定理有

$$\int_V(\mathrm{div}\boldsymbol{E}-\rho/\varepsilon_0)\mathrm{d}V=0$$

由于这对于任意体积 V 都成立,从而

$$\mathrm{div}\boldsymbol{E}=\rho/\varepsilon_0 \qquad [14]$$

按照类似的精神论证,我们也可以证明固定不动的电荷分布的电场是保守的,其意义是当一电荷沿一闭合回路移动,场所做的总功为零,即对任意闭合路径,有

$$\oint\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{s}=0$$

这等价于

$$\mathrm{curl}\boldsymbol{E}=0 \qquad [15]$$

因为根据斯托克斯定理,

$$\oint\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{s}=\int_S\mathrm{curl}\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}$$

式中,S 是以路径为边界的任意曲面,[15]成立当且仅当,对于一切可能的路径和一切可能的 S,积分为零。

单个固定不动电荷的场是保守的,因为

$$\boldsymbol{E}=-\mathrm{grad}\phi,\ \phi=\frac{e}{4\pi\varepsilon_0 r}$$

由于梯度的旋度恒为零,因此 $\mathrm{curl}\boldsymbol{E}=0$。对于连续分布,$\boldsymbol{E}=-\mathrm{grad}\phi$,式中

$$\phi(\boldsymbol{r})=\frac{1}{4\pi\varepsilon_0}\int_{r'\in V}\frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{d}V' \qquad [16]$$

在此积分中,$\boldsymbol{r}$(求 ϕ 值之点的位置)是固定的,积分遍及各个电荷的位置 $\boldsymbol{r}'$,不管在 $\boldsymbol{r}=\boldsymbol{r}'$ 的奇异性,积分有很好的定义,所以[15]对于固定不动电荷的连续分布也成立。

磁场的散度

我们可采用相同的论证,建立慢运动电荷磁场的高斯定理,在这里,

$$\boldsymbol{B}=\frac{\mu_0 e\boldsymbol{v}\wedge\boldsymbol{r}}{4\pi r^3}$$

式中,$\boldsymbol{r}$ 是从电荷到所测场点的矢量。因为 $\boldsymbol{r}/r^3=-\mathrm{grad}(1/r)$,我们有

$$\mathrm{div}\left(\boldsymbol{v}\wedge\frac{\boldsymbol{r}}{r^3}\right)=\boldsymbol{v}\wedge\mathrm{curl}\left(\mathrm{grad}\frac{1}{r}\right)=0$$

所以如同电场情形,除了在 $r=0$ 外,$\mathrm{div}\boldsymbol{B}=0$。然而在磁场的情形,场遍及包围电荷的曲面所做的积分也为零,因为如果 S_R 是中心在电荷处半径为 R 的球,则

$$\int_{S_R}\boldsymbol{B}\cdot\mathrm{d}\boldsymbol{S}=\frac{\mu_0 e}{4\pi}\int_{S_R}\frac{\boldsymbol{v}\wedge\boldsymbol{r}}{r^3}\cdot\frac{\boldsymbol{r}}{r}\mathrm{d}S=0$$

根据散度定理,对于包围电荷的任意曲面同样是正确的,我们推演出如果磁场仅被运动电荷所激发,则对任意体积 V 有

$$\int_{\partial V} \boldsymbol{B} \cdot \mathrm{d}\boldsymbol{S} = 0$$

从而得

$$\mathrm{div}\boldsymbol{B} = 0 \qquad [17]$$

当然,如同电荷激发电场,如果存在激发磁场的自由"磁极",则此式将不成立;类似于[14]中的电荷密度,此方程的右边应有"磁极密度"。

与伽利略相对性的不一致

我们主要关心的是电磁学定律与相对性原理的相容性。正如爱因斯坦观察到的,简单的电磁相互作用确实仅依赖于相对运动;一个导体通过磁体的场运动所感应的电流等同于磁体以相同的相对速度运动越过在固定不动的导体上所激发的电流(爱因斯坦,1905)。很遗憾,这一对称性没有反映在我们的基本原理中。如果假设它在各个惯性参考系中都成立,那么我们可很快消除许多矛盾。

如下的一个情况。一个观察者 O 通过测定相对于电荷的速度为 $\boldsymbol{v}$ 的标准电荷粒子所受的力,依照洛伦兹力定律,

$$\boldsymbol{f} = e(\boldsymbol{E} + \boldsymbol{v} \wedge \boldsymbol{B})$$

他可以测量一点的 $\boldsymbol{B}$ 和 $\boldsymbol{E}$ 值。第二个观察者 O' 相对于第一个观察者以速度 $\boldsymbol{v}$ 运动,将观察到相同的力,但是现在是作用在一个静止粒子上。所以他将测量到电场为 $\boldsymbol{E}' = \boldsymbol{f}/e$。由此得出结论,以速度 $\boldsymbol{v}$ 通过磁场 $\boldsymbol{B}$ 和电场 $\boldsymbol{E}$ 运动的观察者看到的电场

$$\boldsymbol{E}' = \boldsymbol{E} + \boldsymbol{v} \wedge \boldsymbol{B} \qquad [18]$$

交换两个观察者的角色,我们还有

$$\boldsymbol{E} = \boldsymbol{E}' - \boldsymbol{v} \wedge \boldsymbol{B}' \qquad [19]$$

式中,$\boldsymbol{B}'$ 是第二个观察者所测到的磁场。如果两者都成立,则 $\boldsymbol{B}-\boldsymbol{B}'$ 应等于 $\boldsymbol{v}$ 的标量倍数。

但是这与电磁基本原理 3 不相容,如果场是静止点电荷相对于第一观察者的场,则 $\boldsymbol{E}$ 由[7]给出,且

$$\boldsymbol{B} = 0$$

另一方面,第二观察者看到点电荷以速度 $-\boldsymbol{v}$ 运动的场,所以

$$\boldsymbol{B}' = -\frac{\mu_0 e \boldsymbol{v} \wedge \boldsymbol{r}}{4\pi r^3}$$

因此 $\boldsymbol{B}-\boldsymbol{B}'$ 是垂直于 $\boldsymbol{v}$,而不是与它平行。

这一显而易见的矛盾可以解决,部分地,应认识到电磁基本原理 3 是不严格的,它仅当速度足够小到两个粒子之间的磁力与静电力比较可忽略才成立。如果 v 是一个这种典型的速度,则条件是 $v^2\mu_0$ 应远小于 $1/\epsilon_0$,即涉及的速度必须远小于

$$c = \frac{1}{\sqrt{\epsilon_0 \mu_0}} = 3 \times 10^8 \mathrm{m} \cdot \mathrm{s}^{-1}$$

当然,这就是光速。

伽利略不变性的限度

现在我们必须认为电磁基本原理 1～3 是近似的,它们描述粒子和场的相互作用是当粒子相对于彼此运动在速率上远小于光速,特别地应该强调,我们不能预期对粒子以可与 c 比拟的速率运动时电磁基本原理 3 仍成立,我们必须代之以

电磁基本原理 3′ 一个以速度 $\boldsymbol{v}$ 运动的电荷,这里 $v \ll c$,它激发一个磁场

$$\boldsymbol{B} = \frac{\mu_0 e \boldsymbol{v} \wedge \boldsymbol{r}}{4\pi r^3} + O(v^2/c^2) \qquad [20]$$

电荷系统的磁场在一般运动中满足

$$\mathrm{div}\boldsymbol{B} = 0 \qquad [21]$$

其次,我们保留了[21]作为表述的微分形式,即不存在自由磁极;磁场仅由电荷的运动激发。做了这一变更,只要我们忽略 v^2/c^2 级项,理论就与相对性原理就会和谐一致。以电磁基本原理 3′替代电磁基本原理 3 解决了显而易见的矛盾;只要速度远小于光速,爱因斯坦指出的导体在磁场中运动激发的电流和磁体越过导体的运动所激发的电流之间的对称性就可被解释。

然而主要的问题仍存在,电磁学方程组在速度与 c 可比拟的伽利略变换下不是不变的。这一矛盾仍然存在,但是它比原先出现的更加微妙。有三条可能的出路:(1)非不变性是实在的,有可观察的效应(必需有 v^2/c^2 级或更小级),(2)麦克斯韦理论是错误的,或(3)伽利略变换是错误的,意想不到的是物理学采取最后一条路。然而还是跳过这故事向前,我们的任务是导出麦克斯韦方程组。

法拉第感应定律

慢运动电荷的磁场总是小于它的相关电场(即使我们用 $c\boldsymbol{B}$ 代替 $\boldsymbol{B}$ 并使用与 $\boldsymbol{E}$ 相同的单位)。然而电路中的电流所激发的磁场不会被强大的电场所支配。这是因为在低速下电流是被电子的流动建立起来的,而总的说来,导线中的物质大致是电中性的,带正电的核的电场与带负电的电子的电场相抵消。

这是下面从速度远小于 c 的伽利略不变性导出法拉第感应定律应铭记的物理脉络,这一定律涉及沿电路的电动势或"电压"与遍及电路作为边界的曲面上的磁场 $\boldsymbol{B}$ 的变化率。用它的微分形式,定律变为麦克斯韦方程组之一。

首先假设场被电荷激发,电荷全部相对于给定的惯性参考系 R 并以相同的速度 $\boldsymbol{v}$ 运动,于是在相对于 R 以速度 $\boldsymbol{v}$ 运动的第二个参考系 R' 中存在电荷固定不动的分布。如果速度远小于光速,则 R' 内测得的电场 $\boldsymbol{E}'$ 与 R 内测得的电场 $\boldsymbol{E}$ 和磁场 $\boldsymbol{B}$ 有关,有

$$\boldsymbol{E}' = \boldsymbol{E} + \boldsymbol{v} \wedge \boldsymbol{B}$$

由于 R' 内测得的场是固定不动的电荷分布的场,有

$$\mathrm{curl}\boldsymbol{E}' = 0$$

在 R 中,电荷全都以速度 $\boldsymbol{v}$ 运动,因此它们的位形从时刻 t 点 $\boldsymbol{r}$ 到时刻 $t+\tau$ 点 $\boldsymbol{r}+\boldsymbol{v}\tau$ 显示严格相同,因此

$$\boldsymbol{B}(\boldsymbol{r}+\boldsymbol{v}\tau, t+\tau) = \boldsymbol{B}(\boldsymbol{r}, t)$$
$$\boldsymbol{E}(\boldsymbol{r}+\boldsymbol{v}\tau, t+r) = \boldsymbol{E}(\boldsymbol{r}, t)$$

于是取有关 τ 在 $\tau=0$ 的导数

$$\boldsymbol{v}\cdot\mathrm{grad}\boldsymbol{B}+\frac{\partial\boldsymbol{B}}{\partial t}=0$$

$$\boldsymbol{v}\cdot\mathrm{grad}\boldsymbol{E}+\frac{\partial\boldsymbol{E}}{\partial t}=0 \qquad [22]$$

所以我们必定有

$$\begin{aligned}0=\mathrm{curl}\boldsymbol{E}'&=\mathrm{curl}\boldsymbol{E}+\mathrm{curl}(\boldsymbol{v}\wedge\boldsymbol{B})\\&=\mathrm{curl}\boldsymbol{E}+\boldsymbol{v}\mathrm{div}\boldsymbol{B}-\boldsymbol{v}\cdot\mathrm{grad}\boldsymbol{B}\\&=\mathrm{curl}\boldsymbol{E}+\frac{\partial\boldsymbol{B}}{\partial t}\end{aligned} \qquad [23]$$

式中用到 $\mathrm{div}\boldsymbol{B}=0$。由此可见

$$\mathrm{curl}\boldsymbol{E}+\frac{\partial\boldsymbol{B}}{\partial t}=0 \qquad [24]$$

方程[24]对 $\boldsymbol{B}$ 和 $\boldsymbol{E}$ 是线性的;相对于 R 以不同速度运动的不同的电荷流的磁场和电场相加起来,我们就得到对于运动电荷所激发的电场和磁场,此式普遍成立。

方程[24]可称为法拉第电磁感应定律,它描述了磁场变化如何激发电流,在静态情形下,

$$\frac{\partial\boldsymbol{B}}{\partial t}=0$$

方程化为 $\mathrm{curl}\boldsymbol{E}=0$,此即静电场是保守的条件;也就是说,当电荷沿一闭合路径运动,不存在净功。

更普遍地,考虑一个闭合曲线 γ 形状的导线回路,令 S 是以 γ 为周界的固定曲面,从方程[24]可导出

$$\begin{aligned}\oint_\gamma\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{s}=\int_S\mathrm{curl}\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{S}&=-\int_S\frac{\partial\boldsymbol{B}}{\partial t}\cdot\mathrm{d}\boldsymbol{S}\\&=-\frac{\mathrm{d}}{\mathrm{d}t}\int_S\boldsymbol{B}\cdot\mathrm{d}\boldsymbol{S}\end{aligned} \qquad [25]$$

如果磁场变化导致 $\boldsymbol{B}$ 遍及 S 的积分不是常量,则 $\boldsymbol{E}$ 沿回路的积分不为零,将有一非零的电场沿导线,它将对导线内的电子施以作用力,从而引起电流的流动。

量

$$\oint\boldsymbol{E}\cdot\mathrm{d}\boldsymbol{s}$$

用伏[特]量度,它是当单位电荷绕导线一周电场所做的功。它称为沿电路的电动势,积分联系电路的磁通量,电动势与磁通量变化率之间的关系[25]就是法拉第定律。

匀速运动电荷的场

从这一节的论证,我们可以推出麦克斯韦方程组中的另一个。根据电磁基本原理 3′,速度为 $\boldsymbol{v}$ 的单一电荷 e 激发电场 $\boldsymbol{E}$ 和磁场

$$\boldsymbol{B}=\frac{\mu_0 e\boldsymbol{v}\wedge\boldsymbol{r}}{4\pi r^3}+O(v^2/c^2)$$

式中,$\boldsymbol{r}$ 是从电荷到被测场点的矢量,在电荷静止的参考系 R' 中,它的电场是

$$\boldsymbol{E}'=\frac{e\boldsymbol{r}}{4\pi\varepsilon_0 r^3}$$

在电荷以速度$\boldsymbol{v}$运动的参考系中$\boldsymbol{E}=\boldsymbol{E}'+O(v/c)$,因此

$$c\boldsymbol{B}=\frac{\boldsymbol{v}\wedge\boldsymbol{E}'}{c}=\frac{\boldsymbol{v}\wedge\boldsymbol{E}}{c}+O\left(\frac{v^2}{c^2}\right)$$

两边取旋度,省略v^2/c^2级的项,

$$\begin{aligned}\mathrm{curl}(c\boldsymbol{B})&=\mathrm{curl}\left(\frac{\boldsymbol{v}\wedge\boldsymbol{E}}{c}\right)\\&=\frac{1}{c}(\boldsymbol{v}\mathrm{div}\boldsymbol{E}-\boldsymbol{v}\cdot\mathrm{grad}\boldsymbol{E})\end{aligned}$$

而由[22]

$$\mathrm{div}\boldsymbol{E}=\rho/\epsilon_0,\qquad \boldsymbol{v}\cdot\mathrm{grad}\boldsymbol{E}=-\frac{\partial\boldsymbol{E}}{\partial t}$$

因此

$$\mathrm{curl}(c\boldsymbol{B})-\frac{1}{c}\frac{\partial\boldsymbol{E}}{\partial t}=\frac{1}{c\epsilon_0}\boldsymbol{J}=c\mu_0\boldsymbol{J}$$

式中$\boldsymbol{J}=\rho\boldsymbol{v}$,遍及各粒子速度求和,得

$$\mathrm{curl}\boldsymbol{B}-\frac{1}{c^2}\frac{\partial\boldsymbol{E}}{\partial t}=\mu_0\boldsymbol{J}$$

对任意电荷分布均成立,条件是它们的速度均远小于光速。

麦克斯韦方程组

基本原理连同速度远小于光速下的伽利略不变性假设,允许我们导出连续分布的运动电荷在不同的真空中激发的电场和磁场,满足

$$\mathrm{div}\boldsymbol{E}=\rho/\epsilon_0 \qquad [26]$$

$$\mathrm{div}\boldsymbol{B}=0 \qquad [27]$$

$$\mathrm{curl}\boldsymbol{B}-\frac{1}{c^2}\frac{\partial\boldsymbol{E}}{\partial t}=\mu_0\boldsymbol{J} \qquad [28]$$

$$\mathrm{curl}\boldsymbol{E}+\frac{\partial\boldsymbol{B}}{\partial t}=0 \qquad [29]$$

式中,ρ是电荷密度,$\boldsymbol{J}$是电流密度,$c^2=1/\epsilon_0\mu_0$。这就是麦克斯韦方程组,现代电动力学的基础,它们连同洛伦兹力定律描述了电荷和电磁场的动力学。

我们得到它们是考虑基本电磁过程如何出现在运动参考系中,这是一条不能令人满意的路线,因为我们看到按这种方法,作为演绎基础的原理同速度可与光速相比较下的伽利略不变性是不相容的。麦克斯韦导出它们是分析精心制作的电场和磁场的力学模型,它被看成是传光以太的位移。这也是不能令人满意的,因为这一模型已经抛弃很久远了。它们今天被接受作为电磁学的理论和实际应用基础的理由与这两种论证很少有关。首先它们是自洽的,其次它们以超乎寻常的精度描述了真实的场的行为。

连续方程

方程组是自洽的并不直接明显,给定ρ和$\boldsymbol{J}$作为坐标和时间的函数,麦克斯韦方程组

是 $\boldsymbol{E}$ 和 $\boldsymbol{B}$ 未知分量的两个标量方程和两个矢量方程,对于 6 个未知量总共有 8 个方程,方程数多于未知量数,因此有可能它们实际上是不相容的。

如果我们取方程[29]的散度,得

$$\frac{\partial}{\partial t}(\mathrm{div}\boldsymbol{B}) = 0$$

这与方程[27]是相容的,因此这里没有问题。然而取方程[28]的散度,代入[26]得

$$0 = \mathrm{div}\ \mathrm{curl}\boldsymbol{B} = \frac{1}{c^2}\frac{\partial}{\partial t}(\mathrm{div}\boldsymbol{E}) + \mu_0 \mathrm{div}\boldsymbol{J}$$

$$= \mu_0\left(\frac{\partial \rho}{\partial t} + \mathrm{div}\boldsymbol{J}\right)$$

这给出一个矛盾,除非

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\boldsymbol{J} = 0 \qquad [30]$$

所以 ρ 和 $\boldsymbol{J}$ 的选择不是没有约束的,它们必须被连续方程[30]所关联,这一点只对物理上适当的电荷分布才成立,它是电荷不能创造也不能消灭表述的微分形式。

电荷守恒

为了看出连续方程和电荷守恒之间的联系,让我们考察以曲面 S 为边界的固定体积 V 内的总电荷。如果电荷是守恒的,则在短时间内任何增加或减少必须被电荷通过 S 流入或流出精确平衡。

考虑 S 的小面元 $\mathrm{d}S$ 具有单位外法线,并考虑在时间 t 具有特定电荷 e 和特定速度 $\boldsymbol{v}$ 的全部粒子,假定单位体积的粒子数是 σ(σ 是位置的函数),在 t 和 $t+\delta t$ 之间穿过面元的粒子数等于在时间 t 位于下述体积区

$$|\boldsymbol{v}\cdot\boldsymbol{n}\mathrm{d}S\delta t|$$

内的粒子数,如图 1 所示。它们对通过面元流出电荷的贡献为 $e\sigma\boldsymbol{v}\cdot\mathrm{d}\boldsymbol{S}\delta t$,而 $\boldsymbol{J}$ 在面元处的值是 $e\sigma\boldsymbol{v}$ 遍及 $\boldsymbol{v}$ 和 e 所有可能值之和。因此,遍及 $\boldsymbol{v}$、e 和曲面的面元求和,并通过对连续分布取极限,总的流出率是

$$\int_S \boldsymbol{J}\cdot\mathrm{d}\boldsymbol{S}$$

电荷守恒意味着流出率应等于 V 内总电荷的减少率,即

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho \mathrm{d}V + \int_S \boldsymbol{J}\cdot\mathrm{d}\boldsymbol{S} = 0 \qquad [31]$$

在积分号下微分第一项,并应用散度定理于第二积分得,

$$\int_V\left(\frac{\partial \rho}{\partial t} + \mathrm{div}\boldsymbol{J}\right)\mathrm{d}V = 0 \qquad [32]$$

如果此式对于任意选择的 V 成立,则 ρ 和 $\boldsymbol{J}$ 必须满足连续方程;反过来,连续方程意味着电荷守恒。

位移电流

麦克斯韦方程组的第三方程可写成

$$\mathrm{curl}\boldsymbol{B} = \mu_0\left(\boldsymbol{J} + \varepsilon_0 \frac{\partial \boldsymbol{E}}{\partial t}\right) \qquad [33]$$

在这一形式中,可看成未知磁场 $\boldsymbol{B}$ 依据已知电流分布 $\boldsymbol{J}$ 和电场 $\boldsymbol{E}$ 的方程,当 $\boldsymbol{E}$ 和 $\boldsymbol{J}$ 与 t 无关,则化为

$$\mathrm{curl}\boldsymbol{B} = \mu_0\boldsymbol{J}$$

它确定恒定电流的磁场,在某种程度上麦克斯韦同时代人已经熟知。但是[33]右边它的第二项是新的,它加到 $\boldsymbol{J}$ 上称为真空位移电流

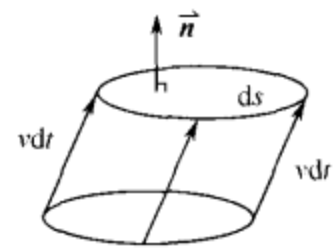

图 1 通过面元的流出量。

$$\varepsilon_0 \frac{\partial \boldsymbol{E}}{\partial t}$$

名称来自类似于绝缘物质中电荷的行为。这里非恒定电流可能流动,但是物质内的电荷分布被外电场扭曲了。当场改变,扭曲也改变,结果显示一种电流,即位移电流,它在改变期间流动。麦克斯韦的远见卓识就是这一相同的项即使在真空中也应存在。结论是深远的,它允许他把光的传播解释为电磁现象。

无源方程组

在远离激发电场和磁场的电荷的真空区内,我们有 $\rho=0=\boldsymbol{J}$,麦克斯韦方程组化为

$$\mathrm{div}\boldsymbol{E} = 0 \qquad [34]$$

$$\mathrm{div}\boldsymbol{B} = 0 \qquad [35]$$

$$\mathrm{curl}\boldsymbol{B} - \frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} = 0 \qquad [36]$$

$$\mathrm{curl}\boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0 \qquad [37]$$

式中,$c=1/\sqrt{\varepsilon_0\mu_0}$,取方程[36]的旋度,代入方程[35]和[37],得

$$0 = \mathrm{grad}(\mathrm{div}\boldsymbol{B}) - \nabla^2\boldsymbol{B} - \frac{1}{c^2}\mathrm{curl}\left(\frac{\partial \boldsymbol{E}}{\partial t}\right)$$

$$= -\nabla^2\boldsymbol{B} - \frac{1}{c^2}\frac{\partial}{\partial t}(\mathrm{curl}\boldsymbol{E}) = -\nabla^2\boldsymbol{B} + \frac{1}{c^2}\frac{\partial^2 \boldsymbol{B}}{\partial t^2}$$

因此,在真空中 $\boldsymbol{B}$ 的 3 个分量满足(标量)波动方程

$$\Box u = 0$$

这里□是达兰贝尔算符,定义为

$$\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} \qquad [38]$$

取方程[37]的旋度,我们也可得$\Box\boldsymbol{E}=0$。

单色平面波

$\boldsymbol{E}$ 和 $\boldsymbol{B}$ 是真空中波动方程矢值解的事实表明:我们找到了麦克斯韦方程组的"平面波"解,其中

$$\boldsymbol{E} = \boldsymbol{\alpha}\cos\Omega + \boldsymbol{\beta}\sin\Omega \qquad [39]$$

式中,$\boldsymbol{\alpha}$、$\boldsymbol{\beta}$ 是常矢量,而

$$\Omega = \frac{\omega}{c}(ct - \boldsymbol{r}\cdot\boldsymbol{e}), \quad \boldsymbol{e}\cdot\boldsymbol{e} = 1 \qquad [40]$$

$\omega>0$,$\boldsymbol{\alpha}$、$\boldsymbol{\beta}$ 和 $\boldsymbol{e}$ 是常量;ω 是频率,$\boldsymbol{e}$ 是给出传播方向的单位矢量(t 增加 τ 且 $\boldsymbol{r}$ 增加 $c\tau\boldsymbol{e}$ 保持 Ω[①] 不变)。这满足波动方程,要不是常量可普遍选取,将不可能找到使方程[34]~[37]也成立的 $\boldsymbol{B}$。

取方程[39]的散度,得

$$\mathrm{div}\boldsymbol{E} = \frac{\omega}{c}(\boldsymbol{e}\cdot\boldsymbol{\alpha}\sin\Omega - \boldsymbol{e}\cdot\boldsymbol{\beta}\cos\Omega) \qquad [41]$$

因为方程[34]成立,所以必须选择 $\boldsymbol{\alpha}$ 和 $\boldsymbol{\beta}$ 垂直于 $\boldsymbol{e}$。因为方程[37]成立,所以必须找到 $\boldsymbol{B}$ 使

$$\mathrm{curl}\boldsymbol{E} = \frac{\omega}{c}(\boldsymbol{e}\wedge\boldsymbol{\alpha}\sin\Omega - \boldsymbol{e}\wedge\boldsymbol{\beta}\cos\Omega) = -\frac{\partial\boldsymbol{B}}{\partial t} \qquad [42]$$

一种可能的选择是

$$\boldsymbol{B} = \frac{\boldsymbol{e}\wedge\boldsymbol{E}}{c} = \frac{1}{c}(\boldsymbol{e}\wedge\boldsymbol{\alpha}\cos\Omega + \boldsymbol{e}\wedge\boldsymbol{\beta}\sin\Omega) \qquad [43]$$

不难看出 $\boldsymbol{E}$ 和 $\boldsymbol{B}$ 则同样满足[35]和[36]。

这种方法得到的解称为“单色平面电磁波”。

注意,$\boldsymbol{E}$ 和 $\boldsymbol{B}$ 垂直于传播方向,在此意义下这样的波是横波,$\boldsymbol{E}$ 的定义可更简要地写成如下形式,

$$\boldsymbol{E} = \mathrm{Re}[(\boldsymbol{\alpha} + \mathrm{i}\boldsymbol{\beta})\mathrm{e}^{-\mathrm{i}\Omega}] \qquad [44]$$

在傅里叶分析中的一个练习就是证明真空中的每一个解是单色平面波的组合。如果 $\boldsymbol{\alpha}$ 和 $\boldsymbol{\beta}$ 成正比,平面波是“平面”偏振的或“线”偏振的;如果 $\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}=\boldsymbol{\beta}\cdot\boldsymbol{\beta}$,$\boldsymbol{\alpha}\cdot\boldsymbol{\beta}=0$,平面波则是“圆”偏振的。

麦克斯韦理论的核心概念是具有确定频率或一定色的光波被用麦克斯韦方程组的单色平面解来表示。

势

对于真空中麦克斯韦方程组的每一个解,$\boldsymbol{E}$ 和 $\boldsymbol{B}$ 的分量满足三维波动方程,但是反过来则是不正确的,也就是说如果

$$\Box\boldsymbol{B} = 0, \quad \Box\boldsymbol{E} = 0$$

则说 $\boldsymbol{E}$ 和 $\boldsymbol{B}$ 满足麦克斯韦方程组,一般是不正确的。发生这种情形,两个场的散度必须为零,同时它们必定被[36]和[37]所关联。如果我们不是用场本身而是用称为“势”的辅助量来处理,这种附加的约束要稍许简单些。

势的定义依赖于矢量微积分里的标准可积条件。假定 $\boldsymbol{v}$ 是依赖于时间的矢量场,如果 $\mathrm{curl}\boldsymbol{v}=0$,则存在一个函数 ϕ 使

$$\boldsymbol{v} = \mathrm{grad}\phi \qquad [45]$$

如果 $\mathrm{div}\boldsymbol{v}=0$,则存在第二个矢量场 $\boldsymbol{a}$ 使

$$\boldsymbol{v} = \mathrm{curl}\boldsymbol{\alpha} \qquad [46]$$

---

① 原文为 u,似有误——译者注。

ϕ 和 $\boldsymbol{a}$ 都不能由 $\boldsymbol{v}$ 惟一确定,一方面,如果[45]成立,则用 $\phi'=\phi+f$ 代替 ϕ,式中 f 仅为时间的函数,它也成立,第二方面,如果[46]成立,则用

$$\boldsymbol{a}' = \boldsymbol{a} + \mathrm{grad}u$$

代替 $\boldsymbol{a}$ 也成立,u 是位置和时间的任意标量函数。应该记住现在的陈述是局域的。如果 $\boldsymbol{v}$ 在拓扑非平凡的区域 U 上有定义,则不可能找到遍及整个 U 均合适的 ϕ 或 $\boldsymbol{a}$。

现在假设给定的场 $\boldsymbol{E}$ 和 $\boldsymbol{B}$ 满足用电荷密度 ρ 和电流密度 $\boldsymbol{J}$ 代表的有源麦克斯韦方程组,因为 $\mathrm{div}\boldsymbol{B}=0$,存在依赖于时间的矢量场 $\boldsymbol{A}(t,x,y,z)$ 使

$$\boldsymbol{B} = \mathrm{curl}\boldsymbol{A}$$

如果将 $\boldsymbol{B}=\mathrm{curl}\boldsymbol{A}$ 代入[29],交换旋度和对时间的导数,则得

$$\mathrm{curl}\left(\boldsymbol{E}+\frac{\partial \boldsymbol{A}}{\partial t}\right)=0$$

由此得出存在一个标量 $\phi(t,x,y,z)$ 使

$$\boldsymbol{E} = -\mathrm{grad}\phi - \frac{\partial \boldsymbol{A}}{\partial t} \qquad [47]$$

这一矢量场 $\boldsymbol{A}$ 称为"磁矢势",使方程[47]成立的函数 ϕ 称为"电标势"。

反过来,给定 t,x,y,z 的标量函数 ϕ 和矢量函数 $\boldsymbol{A}$,可通过

$$\boldsymbol{B} = \mathrm{curl}\boldsymbol{A}, \quad \boldsymbol{E} = -\mathrm{grad}\phi - \frac{\partial \boldsymbol{A}}{\partial t} \qquad [48]$$

定义 $\boldsymbol{B}$ 和 $\boldsymbol{E}$,于是因为

$$\mathrm{div}\boldsymbol{B} = 0, \quad \mathrm{curl}\boldsymbol{E}+\frac{\partial \boldsymbol{B}}{\partial t}=0$$

麦克斯韦方程组中的两式自动成立,剩下的一对方程转变为对 $\boldsymbol{A}$ 和 ϕ 的条件,方程[26]变成

$$\mathrm{div}\boldsymbol{E} = -\nabla^2\phi - \frac{\partial}{\partial t}(\mathrm{div}\boldsymbol{A}) = \frac{\rho}{\varepsilon_0}$$

方程[28]变成

$$\mathrm{curl}\boldsymbol{B} - \frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} = -\nabla^2\boldsymbol{A} + \mathrm{grad}\ \mathrm{div}\boldsymbol{A} + \frac{1}{c^2}\frac{\partial}{\partial t}\left(\mathrm{grad}\phi + \frac{\partial \boldsymbol{A}}{\partial t}\right) = \mu_0\boldsymbol{J}$$

如果令

$$\alpha = \frac{1}{c^2}\frac{\partial \phi}{\partial t} + \mathrm{div}\boldsymbol{A}$$

则可将 $\boldsymbol{A}$ 和 ϕ 的方程改写成更简练的

$$\Box\phi - \frac{\partial \alpha}{\partial t} = \frac{\rho}{\varepsilon_0}$$

$$\Box\boldsymbol{A} + \mathrm{grad}\alpha = \mu_0\boldsymbol{J}$$

这里我们对 4 个未知量(ϕ 和 $\boldsymbol{A}$ 的分量)有 4 个方程(一个标量方程,一个矢量方程)。任意一组解 ϕ,$\boldsymbol{A}$ 通过[48]确定麦克斯韦方程组的一个解。

规范变换

给定麦克斯韦方程组的解 $\boldsymbol{E}$ 和 $\boldsymbol{B}$,在 $\boldsymbol{A}$ 和 ϕ 的选择上还有什么自由度? 首先,$\boldsymbol{A}$ 被

curl$\boldsymbol{A}=\boldsymbol{B}$ 确定到可用

$$\boldsymbol{A}' = \boldsymbol{A} + \mathrm{grad}u$$

替代 $\boldsymbol{A}$,其中 u 是位置和时间的函数。相应于 $\boldsymbol{A}'$的标势 ϕ'必须选择使

$$-\mathrm{grad}\phi' = \boldsymbol{E} + \frac{\partial \boldsymbol{A}'}{\partial t} = \boldsymbol{E} + \frac{\partial \boldsymbol{A}}{\partial t} + \mathrm{grad}\left(\frac{\partial u}{\partial t}\right)$$

$$= -\mathrm{grad}\left(\phi - \frac{\partial u}{\partial t}\right)$$

也就是说,$\phi' = \phi - \partial u/\partial t + f(t)$,式中 f 仅为 t 的函数,我们可以通过减去

$$\int f \mathrm{d}t$$

把 f 吸收到 u 中(这不改变 $\boldsymbol{A}'$),所以在选择 $\boldsymbol{A}$ 和 ϕ 的自由度是对任意的 $u=u(t,x,y,z)$ 取变换

$$\boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \mathrm{grad}u,\ \phi \to \phi' = \phi - \frac{\partial u}{\partial t} \qquad [49]$$

变换[49]称为“规范变换”。

在变换[49]下

$$\alpha \to \alpha' = \frac{1}{c^2}\frac{\partial \phi'}{\partial t} + \mathrm{div}\boldsymbol{A}' = \alpha - \Box u$$

在关于 α 相当温和的条件下,可以证明非齐次波动方程

$$\Box u = \alpha \qquad [50]$$

有解 $u=u(t,x,y,z)$。如果选择 u 使[50]成立,则被变换的势 $\boldsymbol{A}'$和 ϕ'满足

$$\mathrm{div}\boldsymbol{A}' + \frac{1}{c^2}\frac{\partial \phi'}{\partial t} = 0$$

这就是在 L Lorenz 之后被命名的“洛伦茨规范条件”[①](不是“洛伦兹收缩”的 H A Lorentz)。

如果我们要求洛伦茨条件,在选择 $\boldsymbol{A}$ 和 ϕ 上惟一剩下的自由度是作规范变换[49],其中 u 是波动方程$\Box u=0$ 的解。在洛伦茨条件下,麦克斯韦方程组取如下形式

$$\Box\phi = \rho/\varepsilon_0,\ \Box\boldsymbol{A} = \mu_0\boldsymbol{J} \qquad [51]$$

与洛伦茨条件的相容性可根据 ρ[②] 和 $\boldsymbol{J}$ 的连续方程得出。

所以在无源情形下,关于势的麦克斯韦方程组在洛伦茨规范下化为

$$\Box\phi = 0, \Box\boldsymbol{A} = 0 \qquad [52]$$

以及约束

$$\mathrm{div}\boldsymbol{A} + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0$$

例如,我们可选择矢势分量的标量波动方程的 3 个任意解,从而用

$$\phi = c^2\int \mathrm{div}\boldsymbol{A}\mathrm{d}t$$

来定义 ϕ。不管我们取怎样的选择,我们将获得麦克斯韦方程组的一个解,并且麦克斯韦

① 此为作者的新见解,以前各种书籍都把它称为“洛伦兹规范条件”——译者注。

② 原文为 ϕ,似有误——译者注。

方程组(无源的)的每一个解都是由某个这种选择引起的。

历史性注记

18 世纪末,人们已经知道四类电磁现象,但还不知晓它们之间的联系:

- 磁,希腊语关于"来自玛格尼西亚之石"转意而来的词。
- 静电,琥珀与毛皮摩擦产生,"电"这个词来自希腊语的"琥珀"。
- 光。
- 伽伐尼状态或"动物电",L. 伽伐尼发现的电池所产生的电。

统一理论的构建是漫长而艰苦的事业。现在回顾起来,似乎古怪的各种各样的企图阻挠了对电磁学的理解,而它是用创造如"电流体"、"磁涡旋"的力学模型来表述的,我们可看到,到爱因斯坦 1905 年的论文为结束,这个时期的遗产在现代术语库中仍继续存在误导的和已不通用的术语有"磁通量"、"力线"、"电位移"等。

麦克斯韦的贡献是决定性的,即使我们现在称为"麦克斯韦理论"的说法,许多是他的继承者(洛伦兹、赫兹、爱因斯坦等人)的缘故;正如我们看到,在麦克斯韦自己描述的电磁学中的关键成分是"电磁以太",一种被假定传播电磁波的弥漫介质,它被爱因斯坦摈弃了。

粗略的年表如下:

- 1800 年 伏打演示了伽伐尼状态与静电的联系。
- 1820 年 奥斯特显示了电池的电流引发对磁体的作用力。
- 1822 年 安培建议光是两类电流体组成的"传光以太"中的波动。同年,伽利略的《关于两大世界体系的对话》从被禁书目中解禁。
- 1831 年 法拉第显示运动磁体可感应电流。
- 1846 年 法拉第建议光是磁力线中的振动。
- 1863 年 麦克斯韦发表了描述电场和磁场动力学的方程组。
- 1905 年 爱因斯坦的论文"论动体的电动力学"。

进一步的阅读材料

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导论:平衡态统计力学

基础:原子与分子

经典统计力学研究粒子、原子和分子宏观集合的性质,而且假定集合中的粒子是点粒子,服从经典力学。宏观系统与微观系统之间的差异是逐渐消失的,事实上,统计力学的基础建立在少体粒子系统(被证实或假定)的性质之上。

宏观系统通常被认为处在平稳态,这意味着它的微观构形随时间一个接一个的演化,但宏观看起来是一样。观测时间演化与用同一方式对系统(时间"不要太靠近")的独立副本取样是一样的。

一个必要的基本区别是:一个平稳态可能处在或不处在平衡态。当粒子被围在一个容器 Ω 内,且只受到粒子间的守恒相互作用以及可能外部守恒力的作用,第一种情况就会出现:在一个容器中,除了内部相互作用,还受到容器 Ω 壁和重力作用的气体是一个典型的例子,这是一类非常受限制的系统和状态。

一个更加一般的情形是,系统处于平稳态,但它还受到非守恒力的作用:一个典型的例子是,有一轮子在其中旋转的气体或者液体,就像在焦耳实验中,通过一些装置的作用保持温度恒定,这个装置被称为恒温器。在统计力学中,这种装置必须由包括非守恒力在内的某种力来模仿,这些力防止由外部力向系统传输某种能量——这种能量传输会阻止平稳态的出现。例如,恒温器可简单看作是一个不变的摩擦力(如在被搅拌的不可压缩液体,或由电动势在其中产生循环电流的导线)。

一个更为基础的方法,是设想恒温器不是一唯象引入的非守恒力(例如,摩擦力),而是归结为与处于"无限平衡"的一个外部无限大系统的相互作用。

在任何一个事件中,非平衡平稳态内在地比平衡态更加复杂。这里注意力将局限于关注围在立方盒子 Ω 中 N 个全同点粒子 $\boldsymbol{Q}=(\boldsymbol{q}_1,\cdots,\boldsymbol{q}_N)$ 系统的平衡态统计力学。立方盒子 Ω 的体积为 V、边长为 L,通常假定具有完全反射壁。

质量为 m、位于 $\boldsymbol{q},\boldsymbol{q}'$ 的粒子按照对势能 $\varphi(\boldsymbol{q}-\boldsymbol{q}')$ 发生相互作用。微观运动遵守方程:

$$m\ddot{\boldsymbol{q}}_i=-\sum_{j=1}^{N}\partial_{q_i}\varphi(\boldsymbol{q}_i-\boldsymbol{q}_j)+\sum_i W_{\text{wall}}(\boldsymbol{q}_i)\overset{\text{def}}{=}-\partial_{q_i}\Phi(\boldsymbol{Q}) \qquad [1]$$

其中势能 φ 被假定是光滑的(除了在 $|\boldsymbol{q}_i-\boldsymbol{q}_i'|\leqslant r_0$ 势能 φ 可能达到 $+\infty$),这就是说,粒子不可能达到比 r_0 更近的距离;在式[1]的情况被解释为设想粒子经历了弹性碰撞。势能 W_{wall} 用来模仿容器,除非明确的说明,它将由一个弹性碰撞规则来代替。

所以,时间演化 $(\boldsymbol{Q},\dot{\boldsymbol{Q}})\to S_t(\boldsymbol{Q},\dot{\boldsymbol{Q}})$ 将在 N 粒子位置-速度空间 $\hat{F}(N)$ 中被描述,或更方便地在相空间中,即在动量-位置($\boldsymbol{P},\boldsymbol{Q}$,而 $\boldsymbol{P}=m\dot{\boldsymbol{Q}}$)空间 $\mathcal{F}(N)$ 中的时间演化 S_t 描述。这种运动是守恒的,其能量

$$U\overset{\text{def}}{=}\sum_i\frac{1}{2m}\boldsymbol{p}_i^2+\sum_{i<j}\varphi(\boldsymbol{q}_i-\boldsymbol{q}_j)+\sum_i W_{\text{wall}}(\boldsymbol{q}_i)\overset{\text{def}}{=}K(\boldsymbol{P})+\Phi(\boldsymbol{Q})$$

为一运动常数。如果容器壁是完全反射的,Φ 中的最后一项不存在。这样方便将动力学与两个动力系统联系起来,一个是 $6N$ 维相空间的$(\mathcal{F}(N), S_t)$,另一个是$(6N-1)$维能量为 U 之曲面上的$(\mathcal{F}_U(N), S_t)$。

由于动力系统[1]是相空间中的哈密尔顿系统,其哈密尔顿量为

$$H(\boldsymbol{P},\boldsymbol{Q}) \stackrel{\text{def}}{=} \sum_i \frac{1}{2m} p_i^2 + \phi(\boldsymbol{Q}) \stackrel{\text{def}}{=} K + \phi$$

由此知,体积 $d^{3N}\boldsymbol{P}d^{3N}\boldsymbol{Q}$ 守恒(即一个区域 E 与 S_tE 具有同样的体积),且面积 $\delta(H(\boldsymbol{P},\boldsymbol{Q})-U)d^{3N}\boldsymbol{P}d^{3N}\boldsymbol{Q}$ 同样守恒。

上述动力系统被清楚地定义,即 S_t 是对所有 $t\in(-\infty, \infty)$在相空间中整体定义的映射,条件是相互作用势能为下有界,这被先验地蕴含于能量守恒所导致的界限。对于重力或者库仑相互作用,甚至为了定义关于运动的统计理论所需的关键量,有许多必须说、假定和做。

尽管我们的世界是三维的(或者直到最近的革命性理论至少被相信如此),考虑维数 $d\neq 3$ 粒子系统是有用的。在这种情况下,上面的 $6N$ 和 $3N$ 分别变为 $2dN$ 和 dN。维数 $d=1,2$ 系统实际上有时是细丝或薄膜非常好的模型。由于同样的原因,将空间想象成离散的、粒子只能处在一个格子上,例如格子 $\mathbb{Z}^d$(参考章节"格点模型"),经常是有用的。

更多细节,读者可以参考 Gallavotti(1999)。

压强、温度和功能

起初,伯努利推导理想气体定律,由向容器壁上面积为 dS 表面元单位时间转移的平均动量确定密度 ρ 下的压强,即可观测量 $2mv\rho v\mathrm{d}S$ 的平均值,这里 v 是与 dS 发生碰撞粒子速度的垂直分量。如果 $f(v)\mathrm{d}v$ 是速度垂直分量的分布,$f(\boldsymbol{v})\mathrm{d}^3\boldsymbol{v} \equiv \prod_i f(\boldsymbol{v}_i)\mathrm{d}^3\boldsymbol{v}$,$\boldsymbol{v}=(v_1,v_2,v_3)$是总速度的分布,那么平均动量转移是 $p\mathrm{d}S$,它由下式给出

$$\mathrm{d}S\int_{v>0} 2mv^2\rho f(v)\mathrm{d}v = \mathrm{d}S\int mu^2\rho f(v)\mathrm{d}$$

$$= \rho\frac{2}{3}\mathrm{d}S\int \frac{m}{2}\boldsymbol{v}^2 f(\boldsymbol{v})\mathrm{d}^3\boldsymbol{v} = \rho\frac{2}{3}\left\langle\frac{K}{N}\right\rangle\mathrm{d}S \qquad [2]$$

进一步,$(2/3)\langle K/N\rangle$被确定正比于绝对温度$\langle K/N\rangle \stackrel{\text{def}}{=}$常数$\times(3/2)T$,用现在的符号可以写成$(2/3)\langle K/N\rangle = k_{\mathrm{B}}T$。常数 k_{B} 后来被称为玻耳兹曼常数,至少对所有理想气体这个常数都是相同的。这常数对气体特性的不依赖性是阿伏加德罗定律的结果,这个定律说,在同样温度和压力条件下,相同体积的气体包含相同数量的分子。

通过普适常数 k_{B},在平均动能和温度之间的比例关系事实上成为了一个基本假设,它被推广到所有粒子的集合,气体或不是气体,在所有后来的工作中从来没有被质疑(直到量子力学,那里这个假设不再正确,参考章节"量子统计力学")。

更多细节,读者可以参考 Gallavotti(1999)。

热与熵

在克劳修斯发现熵之后,为了用力学解释它,玻耳兹曼引入了热学定理,在 1866 年到 1884 年之间他将其发展到完全一般的情形。与前面提到的热力学温度与平均动能等价

一起,热学定理也可被当作统计物理的一块基石。

这个定理以极大的一般性使得时间和状态平均的概念变得精准,对于给定的任何一个力学系统,它的动力学与 4 个量 U,V,p,T 联系起来,这四个量由合适的力学可观测量(即相空间中的函数)的时间平均来定义,使得外部条件无限小变化时,U,V 分别变化 $\mathrm{d}U$ 和 $\mathrm{d}V$,且比率 $(\mathrm{d}U+p\mathrm{d}V)/T$ 是正合的,即它正好等于一个函数 $S(U,V)$ 相应的变分。为了考虑非常大系统($V\to\infty$),用内蕴量 $u\overset{\text{def}}{=}U/N$ 和 $v=V/N$,可以更好地将这个关系写成

$$(\mathrm{d}u+p\mathrm{d}v)/T \text{ 是正合的} \qquad [3]$$

即它正好等于 $s(U/N,V/N)\equiv(1/N)S(U,V)$ 的变分 $\mathrm{d}s$。

这个证明最初涉及单循环系统,即所有运动是周期性的系统,这个假设明显太局限了。发展到对一般系统的证明,是从早期的"非周期性运动可看作具有无限周期的周期运动"(1866),到后来的遍历假设,到最终意识热学定理并不真正依赖遍历的假设(1884)。

尽管对于一维系统,热学定理证明只是一个简单的检验,但它是一个真正的突破,因为它引出了一般问题的答案,即在什么条件下能够定义力学量,它的变分被约束的满足式[3],因此能被解释为克劳修斯宏观热力学的力学模型。这将被重新在下面导出。

考虑一个一维系统,它受到约束势 $\varphi(x)$ 对应的力作用。对于 $|x|>0$,$|\varphi'(x)|>0$,$\varphi''(0)>0$ 和 $\varphi(x)\xrightarrow[x\to\infty]{}+\infty$。所有的运动都是周期性的,因此系统为单循环系统。假定势能 $\varphi(x)$ 依赖于一个参数 V,定义具有给定能量 U 和给定 V 的运动为一个状态,令

$$\begin{aligned} U &= \text{系统总能量} \equiv K+\Phi \\ T &= \text{动能 } K \text{ 的时间平均} = \langle K\rangle \\ V &= \varphi \text{ 被假定依赖的参数} \\ p &= -\partial V_\varphi \text{ 的时间平均},\ -\langle \partial V_\varphi\rangle \end{aligned} \qquad [4]$$

一个状态由参数 U,V 描述。如果这些参数分别变化 $\mathrm{d}U,\mathrm{d}V$,以及 $\mathrm{d}L\overset{\text{def}}{=}-p\mathrm{d}V$,$\mathrm{d}Q\overset{\text{def}}{=}\mathrm{d}U+\mathrm{d}V$,那么式[3]成立。实际上,令 $x_\pm(U,V)$ 为给定 U,V 的运动的振动极点,并将 S 定义为

$$\begin{aligned} S &= 2\log\int_{x_-(U,V)}^{x_+(U,V)}\sqrt{(U-\varphi(x))}\,\mathrm{d}x \\ &= \mathrm{d}S = \frac{\int(\mathrm{d}U-\partial_{V\varphi}(x)\mathrm{d}V)(\mathrm{d}x/\sqrt{K})}{\int(\mathrm{d}x/\sqrt{K})K} \end{aligned} \qquad [5]$$

注意 $\mathrm{d}x/\sqrt{K}=\sqrt{2/m}\,\mathrm{d}t$,由于对 $\mathrm{d}x/\sqrt{K}$ 积分并除以 $1/\sqrt{K}$ 的积分给出时间平均,可以得到式[3]。

更多细节,读者可以参考 Boltzmann(1968b)和 Gallavotti(1999)。

热学定理和遍历假设

玻耳兹曼试图将结果扩展到一维系统(例如,对于开普勒运动,它并非是单循环,除非仅考虑固定离心率的运动)以外。然而,早期的陈述"非周期性运动可被看作具有无限周期的周期运动",确实是将单循环系统热学定理应用到盒子中非常复杂的气体的核心。

设想气体容器 Ω 由截面为 A 的活塞所密封,活塞作为一个盖子位于原点右端距离为

L 的位置,因此体积为 $V=AL$。如果 $x=(\xi,\eta,\zeta)$ 是粒子的坐标,势能 $\bar{\varphi}(L-\xi)$ 将是活塞的微观模型。当 $r>r_0$,且 $r_0\ll L$,函数 $\bar{\varphi}(r)$ 变为 0,而当 $r=0$ 时函数 $\bar{\varphi}(r)$ 趋向于 $+\infty$。因此,r_0 是活塞附近层的宽度,随机游走到此处的粒子能感受到壁的力。

壁对于总势能 Φ 的贡献 $W_{\text{wall}}=\sum_j\bar{\varphi}(L-\xi_j)$,且 $\partial_V\bar{\varphi}=A^{-1}\partial_L\bar{\varphi}$;假定单循环性,必须估算时间平均 $\partial_L\Phi(x)=\partial_L W_{\text{wall}}\equiv\sum'_j(L-\xi_j)$。随着时间的演化,距离壁小于 r_0 层中的粒子 x_j 且具有分量 ξ_j,它会感受到壁的力并弹回来。层内一个粒子对 $\partial_L\Phi(x)$ 平均的贡献为

$$\frac{1}{\text{总时间}}\,2\int_{t_0}^{t_1}-\bar{\varphi}'(L-\xi_j)\,\mathrm{d}t \qquad [6]$$

这里 t_0 是粒子 j 进入器壁层的第一个瞬间;t_1 是速度的 ξ 分量相对于器壁为零的瞬间。因为 $-\bar{\varphi}'(L-\xi_j)$ 是力的 ξ 分量,当然若是 $\xi_j>0$,这个积分是 $2m|\xi_j|$(通过牛顿定理)。

假定在壁的势能范围内粒子之间没有发生碰撞,如平均自由程远远大于器壁势能 $\bar{\varphi}$ 的范围。因此,单位时间由于对器壁的碰撞产生的平均动量转换由下式给出

$$\int_{v>0}2mvf(v)\rho_{\text{wall}}Av\,\mathrm{d}v,$$

参见式[2]。如果 ρ_{wall},$f(v)$ 分别是器壁附近平均密度和垂直于器壁速度分量在 v 和 $v+\mathrm{d}v$ 之间粒子比例的平均。这里 p,f 被假定与器壁上的位置无关,除了大小为 $o(A)$ 的修正以外,这是正确的。

因而每个粒子和每个速度分量的平均动能可以写成,$\int(m/2)v^2f(v)\mathrm{d}v$,如同 $(1/2)\beta^{-1}$(与式[2]比较),可以得到

$$p\overset{\text{def}}{=\!=}-\langle\partial_v\Phi\rangle=\rho_{\text{wall}}\beta^{-1} \qquad [7]$$

这是压强的物理解释。$(1/2)\beta^{-1}$ 是每个自由度的平均动能:因此它与热力学温度 T 成正比(比较:参考"压力、温度和动能"章节)。

另一方面,如果能量面上的运动以单一周期轨道进行,式[7]中的 p 是一个使得热学定理有效的正确物理量,参见式[4]。因此,将每个能量面上的轨道都看作周期性的(即系统是单循环的)可以导出热学定理,使得 p,U,V,T 都有与其名称对应的物理解释。这表明单循环系统给出了热力学行为的一个自然模型。

为了实际需求,假定一个像体积为 V 容器中气体的混沌系统满足上面的性质,p 可以这样被定义,使得 $\mathrm{d}U+p\mathrm{d}V$ 成为作为积分因子的平均动能 $\langle K\rangle$ 的倒数,进一步 p,U,V,$\langle K\rangle$ 分别具有压力、能量、体积与(除了比例系数的)热力学温度的物理解释。

玻耳兹曼的不连续空间(和时间)概念使得他设想能面是由属于一个单轨道的点组成,如果相空间真正是连续的,这个性质是不可能的。将相空间看作由有限个具有有限体积 $b^{\mathrm{d}N}$ 的"胞腔"组成,对某些 $b>0$(而不是点的连续集),允许他无逻辑矛盾地认为,能量面由单轨道组成,所以运动是那些点(实际上是胞腔)的循环排列。

进一步,这意味着观测量 $F(P,Q)$ 的时间平均被确定为能量面上的平均,这可以通过刘维尔分布

$$C^{-1}\int F(P,Q)\delta(H(P,Q)-U)\,\mathrm{d}P\mathrm{d}Q$$

来计算,这里

$$C=\int\delta(H(P,Q)-U)\mathrm{d}P\mathrm{d}Q$$

是一个适当的归一化因子,可以象征性写为

$$\frac{\mathrm{d}t}{T}=\frac{\mathrm{d}P\mathrm{d}Q}{\int\mathrm{d}P\mathrm{d}Q}$$

或者

$$\lim_{T\to\infty}\frac{1}{T}\int_0 F(S_t(P,Q))\mathrm{d}t=\frac{\int F(P',Q')\delta(H(P',Q')-U)\mathrm{d}P'\mathrm{d}Q'}{\int\delta(H(P',Q')-U)\mathrm{d}P'\mathrm{d}Q'}\qquad[8]$$

除了一个零面积集合,对于所有(分段光滑的)观测量 F 和所有能量面上的点,式[8]的有效性被称为遍历假设。

更多的细节,读者可以参考 Boltzmann(1968)和 Gallavotti(1999)。

系综

1884 年,玻耳兹曼终于意识到,对于由式[8]的右端计算的平均,热学定理的有效性独立于遍历假设的成立,即式[8]并不是必要的,因为通过假设公式中涉及的平均由对式[8]右端概率分布的相空间平均来计算,热学定理(如式[3])也可以推导得出。

进一步,如果 T 被确定为平均动能,U 被确定为平均能量,p 被确定为体积为 V 的容器 Ω 壁的单位表面平均力,那么除了式[8],关系式[3]对相空间中的各类概率分布成立。这其中的一些是:

(1)"微正则系综",它是由 $u=U/N,v=V/N$(每个粒子的能量和体积)参数化的式[8]右端的概率分布集合,

$$\mu^{mc}_{\mu,v}(\mathrm{d}\boldsymbol{P},\mathrm{d}\boldsymbol{Q})=\frac{1}{Z_{mc}(U,N,V)}\delta(H(\boldsymbol{P},\boldsymbol{Q})-U)\frac{\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q}}{N!h^{dN}}\qquad[9]$$

这里 h 是一个具有作用量量纲的常数,在前面章节中提到的相空间离散表示中,这个作用量被取为胞腔体积 $h^{\mathrm{d}N}$。所以,对式[9]的积分可以被解释为所有胞腔的(近似)求和,这些胞腔被设想为 N 个不可区分粒子的微观构型(因此有 $N!$ 个)。

(2)"正则系综",是由 $\beta,v=V/N$ 所参数化的概率分布集合

$$\mu^{c}_{\beta,v}(\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q})=\frac{1}{Z_c(\beta,N,V)}\mathrm{e}^{-\beta H(\boldsymbol{P},\boldsymbol{Q})}\frac{\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q}}{N!h^{\mathrm{d}N}}\qquad[10]$$

对正则系统中可以添加更多的系综,如巨正则系综(吉布斯)。

(3)"巨正则系综",它是由 β,λ 参数化的定义在空间 $\mathcal{F}_{gc}=\bigcup_{N=0}^{\infty}\mathcal{F}(N)$ 的概率分布集合

$$\mu^{gc}_{\beta,\lambda}(\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q})=\frac{1}{Z_{gc}(\beta,\lambda,V)}\mathrm{e}^{\beta\lambda N-\beta H(\boldsymbol{P},\boldsymbol{Q})}\frac{\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q}}{N!h^{\mathrm{d}N}}\qquad[11]$$

因此,有几个不同的热力学模型。接受这些模型作为宏观热力学的真实微观描述的关键检验如下:

(1) 热力学平衡的宏观状态与相空间概率分布集合的元素之间的对应,可通过将具有给定热力学函数值的宏观热力学状态,与具有相同对应微观观察量平均值的概率分布

联系起来(也就是,它们的平均值能解释为热力学函数)。

(2) 一旦在不同系综的元素之间建立起正确的联系,也就是,配对(u,v),(β,v),(β,λ)被这样相互联系起来,以至于可以得到

$$H(\boldsymbol{P},\boldsymbol{Q}),V,\frac{2K(\boldsymbol{P})}{3N},\int\delta_{\partial\Omega}(\boldsymbol{q}_1)2m(\boldsymbol{v}_1\cdot\boldsymbol{n})^2\mathrm{d}\boldsymbol{q}_1 \qquad [12]$$

的平均$U,V,k_BT\overset{\mathrm{def}}{=}\beta^{-1},p|\partial\Omega|$的相同值。这里$\delta_{\partial\Omega}(q_1)$是钉在表面$\partial\Omega$上$\boldsymbol{q}_1$的$\delta$函数。那么所有物理上有趣的可观测量至少在热力学极限$\Omega\to\infty$下都相符。利用这种方式,被考虑概率分布集合中的一个元素μ可与系统宏观平衡态的一个状态联系起来。μ依赖于参数,所以它们形成一个系综:它们中每一个都对应一个宏观平衡态,它的热力学函数是微观观测量的恰当平均值,因此是确认μ参数的函数。

评注:"系综"一词常被用来代表被称为系综的个体概率分布。此处的意思似乎更接近于玻耳兹曼1884年论文(换句话说,"系综"经常被指相空间中点的集合,在这个相空间考虑了一个给定的概率分布。这似乎并非原来的意思)。

举例来说,在微正则分布的情况下,这意味着可以将能量、体积、温度和具有特殊能量u与体积v的平衡态压强,通过适当普适常数与式[12]中力学量对$\mu^{mc}_{u,v}(\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q})$积分建立比例关系。具有特殊能量$u$与特殊体积$v$状态的其他热力学观测量的平均值可由它们对$\mu^{mc}_{u,v}$的积分给出。

同样的,可以把能量、体积、温度和具有特殊能量u与特殊体积v平衡态的压强解释为力学量式[12]对正则分布$\mu^{c}_{\beta,v}(\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q})$的平均值,这个正则分布正好有平均特殊能量$u$。具有特殊能量$u$与特殊体积$v$状态的其他热力学观测量平均值由它们对$\mu^{c}_{\beta,v}$的积分给出。通过巨正则分布,也可以给出一个相似的定义来描述热力学平衡。

更多细节,读者可以参考Gibbs(1981)和Gallavotti(1999)。

系综的等价性

玻耳兹曼证明,通过微正则分布或者正则分布计算平均值时,当改变它们的参数(分别是u,v或β,v)而分别导致能量和体积改变时,基本性质[3]依然满足。他同样证明,一旦被表示为u,v(或任一对热力学参数,例如T,v或p,u)的函数,由[3]意味存在的函数s是一样的。对玻耳兹曼证明进一步的查看表明,[3]在正则系综中严格成立。而在微正则系综中,除了$\Omega\to\infty$时趋于零的修正外,[3]也成立。结果,除去这样的修正,两个系综计算的热力学函数相等。另外,吉布斯补充,对巨正则系综同样成立。

当然,并非相空间中平稳态几率分布的每一个集合都能提供一个热力学模型。玻耳兹曼将那种能提供热力学模型的平稳几率分布的集合称为"正规的",而且这种集合中的元素能按上述提到的方式与宏观平衡态对应而产生热力学模型。正规系综主要例子是微正则、正则和以后的巨正则系综。玻耳兹曼和吉布斯不仅证明这三种系综隶属于正规系综,同时还证明它们产生了相同的热力学函数,即它们产生了相同的热力学。

这意味着理论从对遍历假设或单循环假设正确性的验证中解放了出来。而对于这两种假设,前者至今不能在任意一般性的意义上得以证明,后者则显然是错误的,而条件是从字面上理解而不是把相空间视为有限多分立的微小相格构成。如上的讨论同时意味着吉布斯可以将平衡统计力学的问题陈述如下。

问题:研究上述任何一个系综中几率分布集合的性质。

然而,这并不是意味着前述的三种系综在系统无限大的极限条件下穷尽了正规系综中能产生相同热力学模型的系综。具有正规性质系综的丰富性,既导致了热力学的等价力学模型,也自然地解释了与相变现象的联系(参看"相变和边界条件"章节)。

很明显,已引用的结果并没有"证明"热力学平衡被微正则、正则和巨正则系综描述。但是它们清楚地表明,对于大多数系综,可自由度数目独立地使得热力学的力学模型可以清晰的被定义,并将与热力学量之间建立参量自由的,体系独立的物理上重要的关系(例如由[3],$\partial_u(p(u,v)/T(u,v))\equiv\partial_v(1/T(u,v))$)。

遍历假设这一处于热和熵的力学定理之根本地位的假设并没有得以充分证明。天真的人或许会期待通过一定的时间尺度必然看到已达到平衡。这种称为常返时间的时间尺度是至少历经给定能量条件下所有可能微观态的时间。因此,对为什么需要大量的常返时间而不是问题之解释就变得必需。

事实上,常返时间可以在假设相空间离散的条件下估计:为了防御批评者,玻耳兹曼假设动量以$(2mk_BT)^{1/2}$(即平均动量)为单位离散化,而空间以$\rho^{-1/3}$(平均间距)为单位离散化,意味着胞腔体积为h^{3N},这里$h\equiv\rho^{-1/3}(2mk_BT)^{1/2}$。然后他计算出,即使在这样离散化的情况下,$1cm^3$的氢气在通常情况下完成历经全部等能面的时间是宇宙时间的$10^{10^{19}}$倍。事实上,相体积为$\Gamma=(\rho^{-1/3}N(2mk_BT)^{1/2})^N\equiv h^{3N}$,体积$h^{3N}$中的的胞腔数为$\Gamma/(N!h^{3N})\simeq e^{3N}$,需要遍历所有相格的时间将是$e^{3N}\tau_0$,这里$\tau_0$是典型的原子单位,即$10^{-12}S$,但$N=10^{19}$。在这个意义上讲,年轻的玻耳兹曼做出的大胆陈述:"非周期的运动可以看成周期无穷大的周期运动"是更加定量的。

常返时间如此之久以至于与所有目的都无关;不过,热力学微观理论的正确性仍然可以依赖于微观动力学。(正如玻耳兹曼强调的那样)一旦理解为什么我们能够在人类时间尺度(它与常返时间相比是如此之短)上就可以观察到接近平衡甚至观察到平衡本身,那么这就是可以理解的了。这归因于如下性质:即使在N仅仅是适度的巨大时(例如,幂次是10^3而不是10^{19}),在大多数等能面上其平均值能产生(像压力、温度、能量……)宏观热力函数的几个观察量各自取相同的(微观)值。这就暗示了这个值和平均值一致,而且满足热学定理,并且不与常返时间尺度产生任何矛盾。常返时间尺度主要与**通有的观察量**热学化(即达到时间平均值)所需的时间相关:通有的观察量的确将花费很长的时间去"热学化",但无人关注,原因是通有的观察量(如预先指定粒子的益)与热力学无关。

"证明"这个词至此在本文中还没有在数学意义上使用,仅在20世纪60年代,数学严格分析的相关性才被广泛地意识到,也正是在这个时期,首批热力学函数的数值研究才成为可能,而严格结果需要用来验证各种数值模拟的正确性。

更多的细节可以参看Boltzmann(1968a,b)和Gallavotti(1999)。

热力学极限

采用吉布斯公理的观点,可以有趣地发现得到"热学定理与遍历假设"一节引入的三种系综等价性证明所遵循的路径。

初始步骤为,首先给定体积为$V=L^d$立方体盒子Ω,分别考虑在式[9]、式[10]和式[11]中的归一化因子$Z^{gc}(\beta,\lambda,V)$,$Z^c(\beta,N,V)$和$Z^{mc}(U,N,V)$,检查下面的热力学极限的

存在性:

$$\begin{aligned}
\beta p_{gc}(\beta,\lambda) &\overset{\text{def}}{=} \lim_{V\to\infty}\frac{1}{V}\lg Z^{gc}(\beta,\lambda,V)\\
-\beta f_c(\beta,\lambda) &\overset{\text{def}}{=} \lim_{V\to\infty,\frac{N}{V}=\rho}\frac{1}{N}\lg Z^{c}(\beta,N,V)\\
k_B^{-1}s_{mc}(u,\rho) &\overset{\text{def}}{=} \lim_{V\to\infty,N/V=\rho,U/N=u}\frac{1}{N}\lg Z^{mc}(U,N,V)
\end{aligned}\qquad [13]$$

其中密度 $\rho\overset{\text{def}}{=}v^{-1}\equiv N/V$,而不是 v。归一化因子起到一个重要角色,因为它们具有很简单的热力学解释(参照下一小节):它们分别被称作巨正则、正则和微正则配分函数。

毫不奇怪,为了获得式[13]中的极限存在性证明,对粒子间的相互作用势 $\varphi(q-q')$ 做一些假设是必要的,关于 φ 的这些假设虽不具有一般性,但是物理意义很清晰。它们是

(1) 稳定性:即存在一个常量 $B\geqslant 0$,使得对所有 $N\geqslant 0, q_1,\cdots,q_N\in\mathbf{R}^d$ 有 $\sum_{i<j}^{N}\varphi(q_i-q_j)\geqslant -BN$

(2) 缓增性:即存在常量 $R\geqslant 0$ 使得对 $|q-q'|>R$,$|\varphi(q-q')|<B|q-q'|^{-d-\epsilon_0}$。

基本上所有的微观相互作用都满足这两个假设,除了重力和库仑相互作用需要区别对待(会在热力学表现上产生一些不同的结果)。

例如,假设(1)和(2)在如下情况下成立:对一些 $B_0, B_1, \epsilon_0>0, R>r_0$,$|q|<r_0$ 时 $\varphi(q)$ 为 $+\infty$,$|q|>r_0$ 时 $\varphi(q)$ 光滑,$r_0<|q|\leqslant R$ 时 $\varphi(q)>B_0|q|^{-(d+\epsilon_0)}$,$|q|>R$ 时 $|\varphi(q)|<B_1|q|^{-(d+\epsilon_0)}$。简而言之,$\varphi$ 在粒子接近的时候快速发散,在远距离时趋于 0。这种势称为(广义的)勒那得-琼斯势。如果 $r_0>0$,φ 被称作硬核势。如果 $B_1=0$,势的作用范围有限。(对于涉及违反上述稳定性和缓增性的物理含义,参见附录一)。然而,在接下来的讨论中,为了简明性,同时为了篇幅适中,除非明确说明,我们都只考虑 $B_1=0$ 的情况,即

$$\begin{aligned}
&\varphi(q)>B_0|q|^{-(d+\epsilon_0)}, r_0<|q|\leqslant R\\
&|\varphi(q)|\equiv 0, |q|>R
\end{aligned}\qquad [14]$$

有了稳定性和缓增性假设,就可以对式[13]中极限的存在性做出数学证明:在附录二中,第一个的证明被作为这种方法的一个极简单的例子进行了分析。函数 $\beta p_{gc}(\beta,\lambda)$,$-\beta\rho f_c(\beta,\rho)$,$\rho s_{mc}(u,\rho)$ 有一个值得注意的性质,它们都是凸函数。因此,它们在各自的定义域内部是连续的,固定一个自变量以后,至多除去可数例外点关于另外一个变量是可微的。

在相互作用势无硬核($\rho_{\max}=\infty$)的情况中,可以验证,$-\rho f_c(\beta,\rho)$ 当 $\rho\to 0$ 时比 ρ 更慢地趋于 0,当 $\rho\to\infty$ 时比 $-\rho$ 更快地趋于 $-\infty$(在两种情况下都基本正比于 $-\rho\log\rho$)。类似地,在同样的情况中,可以验证 $s_{mc}(u,\rho)$ 当 $u\to u_{\min}$ 时比 $u-u_{\min}$ 更慢地趋于 0,当 $u\to\infty$ 时比 $-u$ 更快地趋于 $-\infty$。从后一个渐近性,以及式[13]中配分函数之间的关系,可以推出

$$\begin{aligned}
Z^{gc}(\beta,\lambda,V) &= \sum_{N=0}^{\infty} e^{\beta,\lambda,N}Z^{c}(\beta,N,V)\\
Z^{c}(\beta,N,V) &= \int_{-B}^{\infty} e^{-\beta U}Z^{mc}(N,U,V)\,dU
\end{aligned}\qquad [15]$$

从上面提到的凸性有

$$\begin{aligned}\beta p_{mc}(\beta,\lambda) &= \max_v(\beta\lambda v^{-1} - \beta v^{-1} f_c(\beta, v^{-1}))\\ -\beta f_c(\beta, v^{-1}) &= \max_u(-\beta u + k_B^{-1} s^{mc}(u, v^1))\end{aligned} \qquad [16]$$

在定义区间内部,或者在区间上它们都可以达到最大值。令 v_{gc},u_c 分别为式[16]达到最大值的点。

注意:量 $e^{\beta\lambda N}\dot{Z}^c(\beta,N,V)/Z^{gc}(\beta,\lambda,V)$ 可以解释为在巨正则分布中计算密度 $v^{-1}=(N/V)$ 的概率。这样,如果式[16]中第一式的最大值是严格的,即它在单一点达到,则 v^{-1} 的值在不包含最大值点 v_{gc}^{-1} 的闭区间中的概率$<e^{-cV}(c>0,V\to\infty)$,与在任意包含 v_{gc}^{-1} 的区间内 v^{-1} 的取值概率可以比较。因此,在 $V\to\infty$ 时,v_{gc} 具有 v 在巨正则分布中的平均值之含义。

同样

$$e^{-\beta uN}Z^{mc}(uN,N,V)/Z^c(\beta,N,V))$$

作为正则分布下能量密度 u 概率的解释表明,如果式[16]中第二式的最大值是严格的,则 u 在不包含最大值点 u_c 的闭区间中的概率$<e^{-cV}(c>0,V\to\infty)$,可与在包含 u_c 的区间中 u 的取值概率相比较。因此,在 $\Omega\to\infty$ 的极限下,u 的在正则分布下的平均值为 u_c。

如果最大值是严格的,则式[16]建立了巨正则密度、正则能量和巨正则参数 λ 之间的联系,或者正则能量、微正则焓和正则参数 β 之间的联系:

$$\lambda = \partial_{v^{-1}}(v_{gc}^{-1} f_c(\beta, v_{gc}^{-1})), k_B\beta = \partial_u s_{mc}(u_c, v^{-1}) \qquad [17]$$

而凸性和最大值的严格性可以推出导数的存在。

因此,为了保证正则系综和微正则系综的等价性,应该用具有参数(β,v)的正则分布和具有参数(u_c,v)的微正则分布相对应;用具有参数(β,λ)的巨正则分布和具有参数(β,v_{gc})的正则分布相对应。

更多细节,请读者参看 Ruelle(1969)和 Gallavotti(1999)。

热力学函数物理解释

极限[13]的存在蕴含了许多有趣的性质。首先是寻找函数 p_{gc},f_c,s_{mc} 和参数 λ,β 物理意义的可能性。

首先注意,任何体积 V 的巨正则系综平均值$\langle K\rangle_{\beta,\lambda}$是$(d/2)\beta^{-1}\langle N\rangle_{\beta,\lambda}$,以至于在巨正则分布中 β^{-1} 正比于温度 $T_{gc}=T(\beta,\lambda)$,且 $\beta^{-1}=k_BT(\beta,\lambda)$。通过如下的讨论,将很有启发地发现 $p(\beta,\lambda)$ 和 λ 的物理意义。

考虑微正则分布 $\mu_{u,v}^{mc}$ 并记关于从$(\boldsymbol{P},\boldsymbol{Q})$和扩展到 $H(\boldsymbol{P},\boldsymbol{Q})=U$ 范围$(\boldsymbol{P},\boldsymbol{Q})$的积分为 $\int^*$,同时 $q_1\in dV$,这里 dV 是包围区域 Ω 的一个无限小体积。然后,由压强 p 的微观定义(见"引言"一节),有如下关系:

$$\begin{aligned}pdV &= \frac{N}{Z(N,U,V)}\int^* \frac{2}{3}\frac{p_1^2}{2m}\frac{d\boldsymbol{P}d\boldsymbol{Q}}{N!h^{dN}}\\ &= \frac{2}{3Z(U,N,V)}\int^* \delta K(\boldsymbol{P})\frac{d\boldsymbol{P}d\boldsymbol{Q}}{N!h^{dN}}\end{aligned} \qquad [18]$$

其中 $\delta=\delta(H(\boldsymbol{P},\boldsymbol{Q})-U)$。式[18]的右边与下式对比

$$\frac{\partial_v Z(U,N,V)dV}{Z(U,N,V)} = \frac{N}{Z(U,N,V)}\int^* \frac{d\boldsymbol{P}d\boldsymbol{Q}}{N!h^{dN}}$$

给出

$$\frac{\partial_V Z\,\mathrm{d}V}{Z} = N\frac{p\,\mathrm{d}V}{(2/3)\langle K\rangle^*} = \beta p\,\mathrm{d}V$$

因为由 $\int^* K\Big/\int^* 1$ 给出的平均 $\langle K\rangle^*$ 在 N 非常大的情况下本质上与微正则系综的平均值 $\langle K\rangle_{mc}$ 是一样的（即一个粒子对束缚在体积 $\mathrm{d}V$ 中是不敏感的）。在 $V\to\infty, V/N=v$ 的极限下，后面的注释和式[17]的第二式一起分别产生了

$$\begin{aligned} k_B^{-1}\partial_v s_{mc}(u,v^{-1}) &= \beta_p(u,v),\\ k_B^{-1}\partial_u s_{mc}(u,v) &= \beta \end{aligned} \qquad [19]$$

注意到 $p\geqslant 0$，而且它不随 v 增加，这是因为 $s_{mc}(\rho)$ 是 $v=\rho^{-1}$ 的凹函数（事实上，由接着式[14]的注释，$\rho s_{mc}(u,\rho)$ 是 ρ 的凸函数，而且一般说来，如果 $\rho g(\rho)$ 是 ρ 的凸函数，则 $g(v^{-1})$ 必然是 $v=\rho^{-1}$ 的凹函数）。

因此，$\mathrm{d}s_{mc}(u,v)=(\mathrm{d}u+p\mathrm{d}v)/T$，考虑 p 和 T 的物理意义（作为压强和温度，见“温度、压强和动能”一节），在热力学里 s_{mc} 便是熵。因此（见式[16]的第二式），$-\beta f_c(\beta,\rho)=-\beta u_c+k_B^{-1}s_{mc}(u_c,\rho)$ 变成了

$$\begin{aligned} f_c(\beta,\rho) &= u_c - T_c s_{\mathrm{mc}}(u_c,\rho)\\ df_c &= -p dv - s_{mc}\,\mathrm{d}T \end{aligned} \qquad [20]$$

由于 u_c 在物理上解释为正则分布 $\mu^c_{\beta,v}$ 的平均能量（见上节），则 f_c 解释为自由能（与热力学中自由能定义 $F=U-TS$ 比较）。

通过式[17]和式[20]

$$\lambda = \partial_{v^{-1}}(v_{gc}^{-1}f_c(\beta,v_{gc}^{-1})) \equiv u_c - T_c s_{mc} + pv_{gc}$$

以及 v_{gc} 的意义是特殊体积 v。对比热力学中化学势的定义 $\lambda V=U-TS+pV$，可得到 λ 的热力学解释是化学势（参看式[16]和式[17]）。同时，巨正则关系

$$\beta p_{gc}(\beta,\lambda) = \beta\lambda v_{gc}^{-1} - \beta v_{gc}^{-1}(-\beta u_c + k_B^{-1}s_{mc}(u_c,v^{-1}))$$

表明 $p_{gc}(\beta,\lambda)\equiv p$，这意味着压强 $p_{gc}(\beta,\lambda)$ 是表示为温度和化学势函数的压强。

为了超越上面启发式的推导，有必要讨论，凸性和变量 u,v 在区间内部达到式[16]和[17]最大值的性质足以将上面的推理变成严格的数学演绎，这意味着给出式[19]作为 $p(u,v)$ 和 $\beta(u,v)$ 的定义，可得到式[20]的第二个方程，以及 $p_{gc}(\beta,\lambda)\equiv p(u_v,v_{gc}^{-1})$。但是式[16]中 v_{gc} 和 u_c 的值并不必是惟一的，凸函数可包含水平线段，所以一般性的结论是最大值将在一个区间里达到。由此，式[16]的最大值不是取在单个点 v_{gc} 而是可能取在整个区间 $[v_-,v_+]$，在那里式[16]的右边取得最大值。同理，对于式[17]的右边也将由在整个区间 $[u_-,u_+]$ 代替单个点 u_c 取得最大值。

凸性意味着式[16]或[17]取最大值的 λ 或 β 在区间取得的机会要比在单个点取得的机会罕见，其解释是：在这种情况下，热力学函数显示了不连续性，相应的现象称为相变（参看下一节）。

更多的细节，读者可以参看 Ruelle(1969)和 Gallavotti(1999)。

相变和边界条件

在前面两节中，关于描述宏观平衡态系综分布元素之间关系的分析，让我们不仅可以

得到热力学的力学模型,而且对于一个给定的系统,这些模型至少在 $\Omega\to\infty$ 的情况下是一致的。此外,通过不同系综相应分布计算出的热力学函数,其等价性可以推广到分布的完全等价性。

如果式[16]在 v_{gc} 或 u_c 中的某一点上达到最大值,等价性应该发生,从某种意义上来说,$\mu^{gc}_{\beta,\lambda}$, $\mu^{c}_{\beta,v}$ 和 $\mu^{mc}_{u,v}$ 之间的对应就可以建立。因此,给定任意一个局部可观测量 $F(\boldsymbol{P},\boldsymbol{Q})$,将其定义为只通过 $\boldsymbol{p}_i,\boldsymbol{q}_i$ 依赖于$(\boldsymbol{P},\boldsymbol{Q})$,且有 $\boldsymbol{q}_i\in\Lambda$,这里 $\Lambda\subset\Omega$ 是一个有限的区域,那么 $F(\boldsymbol{P},\boldsymbol{Q})$的平均值与在极限条件 $\Omega\to\infty$相对应的分布中是一样的。

对应的建立是通过考虑$(\lambda,\beta)\to(\beta,v_{gc})\leftrightarrow(u_{mc},v)$,这里 v_{gc} 是式[16]取最大值的点,$u_{mc}\equiv u_c$ 是式[17]取最大值的点,$v_{gc}\equiv v$(同样见式[19]和[20])。这意味着如果平均值通过分布 $\mu^{gc}_{\beta,\lambda}$,μ^{c}_{β,m_c}, $\mu^{mc}_{u_{mc}v_{mc}}$ 计算出来,则极限

$$\lim_{V\to\infty}\int F(P,Q)\mu^{a}(\mathrm{d}P\mathrm{d}Q)\overset{\mathrm{def}}{=}\langle F\rangle_a$$

(是 a 独立的),其中分别有 $a=gc,c,mc$　　[21]

是一致的。

对式[21]来说,可能会有例外:的确就像发生在值 u,v 上的那样,式[16]或[17]在某一区间取最大值,而不是在孤立的点;但这并没有把它完全否决,通常情况下,这些例外使式[21]不再成立。

然而,无情形使式[21]不成立,这不得不被看作是一个例外。它预示着一个有趣且重要的现象发生。为了正确地理解这一点,我们必需认识到巨正则,正则及微正则中的概率分布显然不是惟一的可以产生热力学模型的概率分布系综集合,即从某种意义上来说,它们如在“系综的等价性”一节中讨论的那样是正规的。我们可以很容易地构想出更多一般性的概率分布统计系综的正规集合族。尤其是:

定义　考虑巨正则、正则和微正则分布及与之相联系的一个能量函数,其势能除容器里面粒子间的相互作用 Φ 外,还包括容器里面的粒子与外面粒子间的相互作用 $\Phi_{\mathrm{in,out}}$,容器外面的粒子与里边的粒子是全同的,但位置固定,不允许移动,因此在容器 Ω 外每个单位体积元 Δ 中,存在有限个不依赖于 Δ 的受限粒子。外部粒子的这种构形被称作固定外部粒子的边界条件。

有这种边界条件的热力学极限是通过考虑巨正则、正则和微正则分布得到的,依据容器 Ω 里的势能函数 $\Phi+\Phi_{\mathrm{in,out}}$ 来建立这些分布,容器 Ω 的体积是递增的,但应该注意,当体积逐渐变大时,要排除那些本应该来到容器里边的固定粒子。在“热力学极限”这一部分中的论据说明,在那里考虑过的 3 个热力学模型定义了相同的热力学函数,我们可以再次利用它得出结论,即(无限的)“新的”热力学模型事实上给出相同的热力学函数和局部可观测量的平均值。而且,可以利用新的配分函数计算出与式[13]相对应的极限值,这个数值与式[13]中的是一致的(也就是说,它们不依赖于边界条件)。

然而,通常可能有这样的情况发生,即对于很多有特殊状态参数的模型,式[21]中的极限值与在新系综里计算出来的类似极限是不一致的,就是说,一些局部可观测量的平均值对于固定粒子边界条件的改变是不稳定的。

各种热力学模型看起来模棱两可的状况,但有一个非常自然的解释:即那些用来描述宏观态的参数,在取值的时候,有可能对应于不同的平衡态,有相同的参数值。当式[16]

在某一个密度区间达到最大值时,不应该就认为微观的热力学模型有任何缺陷;相反,我们不得不想到可能有一些状态拥有相同的 β,λ,它们是可以通过几率分布来识别的,这些几率分布可以从不同类型的边界条件构成的巨正则、正则和微正则分布中得到。

例如,一个高密度的边界条件有可能导致以 β,λ 为参数的高密度平衡态,也就是在式[16]达到最大值时这个区间右端的密度 v_+^{-1},同时利用低密度边界条件,式[21]中的极限值有可能描述在区间左端密度 v_-^{-1} 或区间中间的某个密度下状态的平均值。因此,出现了如下定义。

定义 *以 β,λ 为参数的巨正则分布,当选择不同的固定外部粒子边界条件时,对所有足够大体积的容器 Ω,如果一些局部可观测量 F 的平均值之间的差别远大于一个量 $\delta>0$,我们就说这个系统在 β,λ 处发生相变。这意味着如果式[21]中的极限存在,它将依赖于边界条件并且这些极限值将代表可观测量在"不同相"里面的平均值。当式[21]中的极限对某些 F 依赖于边界条件时,给定 (β,v) 或 (u,v),会在正则和微正则分布中给出相应的定义。*

评注

(1)主要思想是通过固定一个热力学系综,并变化边界条件,我们可以在选定的系综中在给定的参数值下实现系统的所有可能平衡态(例如,在巨正则、正则、微正则系综中分别为 (β,λ),(β,v) 和 (μ,v))。

(2)必须要在热力学极限下定义相变这一通常的认识是错误的:相变的定义并不要求极限 $\Omega\to\infty$。事实上,通过变换边界条件,局部可观察量的平均值会发生至少不依赖于系统尺寸的变化。因此,相变的发生在有限体积下是完全可以观察的:通过变换边界条件,某些变量的平均值发生改变,改变的最小量不倚赖于系统体积,就足以检验上述现象。这是一种平均值对边界条件变换的不稳定性:该不稳定性并不会随边界趋于无穷大而消失,也就是说,对边界的微扰会产生整体效应,并且局部变量的平均值,如果存在的话,将对边界条件产生非平凡的依赖。这也叫作"长程序"。

(3)可以申明,当以上情况发生时,某些其值不依赖于边界条件(如正则分布中的自由能)的热力学函数,对系综参数可能有不连续的微商。这实际上是经常使用的相变的另外定义之一:这两种一阶相变的定义是等价的。然而,很难用它证明给定系统发生了相变。例如,在下面"格点模型"中考虑的一类系统中的液-气相变仍然是一个未解决的问题。

(4)对平衡态系综理论的一个重要统一是:任何系综的所有分布都可用来描述平衡态。一旦确定一个边界条件,某些平衡态就可能不会被系综中的元素描述到。但是,如果所有边界条件都被允许,在一个给定系综中通过变换边界条件,所由的平衡态就都可以实现。

(5)该分析启发我们,通过引入与外部粒子相互作用而增加的势能,对正则、巨正则、微正则系综进行完全平等的考虑。

(6)上述图像仅对特殊的模型类(典型例子是粒子受约束而占据格点以及硬核势系统,$r_0>0$ 的情况,见式[14])进行了严格证明,但有理由相信它是普遍成立的。至少与经典统计力学中目前已知的情况一致。普遍证明的困难在于,需要比固定粒子这样的边条件更复杂的边界条件(比如,在外部放置不同粒子,使之与系统以任意势能而非通过 φ 相互作用)。

在对系综等价性以及边界条件重要性的讨论中已经考虑了许多 $\Omega\to\infty$ 的极限情况,

这种问题时有发生。准确起见,有必要对无穷大体积下的平衡态问题建立一个正式定义:尽管无穷大体积是非物理的一种理想情况,但仍需要定义这样的态,以便对某些概念(比如纯态)可以避开冗繁的描述,用简炼的语言给以定义。因此,

定义 具有无穷大体积的状态,其参数(β,v),μ,v 或 β,λ,是一系列平均值 $F\to\langle F\rangle$,这些平均值是通过对有限尺度时,取一般的边界条件为固定外部粒子,固定参数(β,v),(μ,v)或(β,λ)下,Ω_n 中的正则、微正则或巨正则分布的平均值$\langle F\rangle\Omega_n$取极限$\Omega_n\to\infty$得到的,对所有变量 F 该极限同时存在。

有了无穷大体积状态的定义,我们考虑一个局部变量 $G(X)$,并设 $\tau_\xi G(X)=G(X+\xi)$,$\xi\in R^d$,其中 $X+\xi$ 表示对构型 X 中所有粒子平移 ξ:如果对任意一对局部变量 F,G 满足下式,则该无穷大体积态叫作一个纯态

$$\langle F_{\tau_\xi}G\rangle-\langle F\rangle\langle\tau_\xi G\rangle\xrightarrow[\xi\to\infty]{}0 \qquad [22]$$

此式称作对 F,G 的集团性质。

评注(6)中暗含的结果是,至少在硬核系统(或在"格点模型"一节讨论的简单格点模型)中,无穷大体积平衡态在上面的意义下至少穷尽了无穷大体积纯态的完全性。进一步讲,同样方法得到的其他态是纯态的凸组合,即纯相的"统计混合"。注意,普遍来说,$\langle\tau_\xi G\rangle$不能换为$\langle G\rangle$,因为并不是所有的无穷大体积纯态都一定是平移不变的,简单情形下(如晶体中),甚至有可能所有的平移不变的态都不是纯态。

评注

(1)这意味者,在后一种模型中,对边界条件的推广,例如,考虑外部的粒子与系统内部的不同,采用周期或部分周期边界条件,或者普遍使用引入一个小辅助势实现无穷大体积态,再去掉这个势,并不会使态的集合更加扩大(但有时仍有用:在"连续对称性:$d=2$晶体不存在"一节里,将给出一个例子,通过采用后一种引入小势场的方法研究相变)。

(2)如果 χ 是某一局部事件的示性函数,考虑在无穷大体积态中该事件重复发生的概率(定义其为)$\langle\chi\rangle$是有意义的。在无穷大体积态中可以定义 p-点关联函数为在 $\boldsymbol{x}_1$,$\boldsymbol{x}_2,\cdots,\boldsymbol{x}_p$ 处发现 p 粒子的概率密度。例如,如果该态通过正则态$\langle\cdot\rangle_{\Omega_n}$的极限得到,且对应参数 $\beta,\rho=N_n/V_n$ 以及一系列体积 Ω_n,那么有

$$\rho(\boldsymbol{x})=\lim_n\Big\langle\sum_{j=1}^{N_n}\delta(\boldsymbol{x}-q_j)\Big\rangle_{\Omega_n}$$

$$\rho(\boldsymbol{x}_1,\boldsymbol{x}_2,\cdots\boldsymbol{x}_p)=\lim_n\Big\langle\sum_{i_1,\cdots,j_p}^{N_n}\prod_{j=1}^{p}\delta(\boldsymbol{x}_j-q_{i_j})\Big\rangle_{\Omega_n}$$

其中求和遍及所有有序对$(j_1,\cdots,j_p)$。因此,对关联函数 $\rho(\boldsymbol{q},\boldsymbol{q}')$ 及其可能的集团性质如下

$$\rho(q,q')\overset{\text{def}}{=}\lim_n\frac{\int_{\Omega_n}\exp(-\beta U(\boldsymbol{q},\boldsymbol{q}',\boldsymbol{q}_1,\cdots,\boldsymbol{q}_{N_{n-2}}))\mathrm{d}\boldsymbol{q}_1\cdots\mathrm{d}\boldsymbol{q}_{N_{n-2}}}{(N_{n-2})!Z_0^c(\beta,\rho,V_n)}$$

$$\rho(\boldsymbol{q},(\boldsymbol{q}'+\boldsymbol{\xi}))-\rho(\boldsymbol{q})\rho(\boldsymbol{q}'+\boldsymbol{\xi})\xrightarrow[\xi\to\infty]{} \qquad [23]$$

其中

$$Z_0^c\overset{\text{def}}{=}\int\mathrm{e}^{-\beta U(Q)}\mathrm{d}Q$$

是构形配分函数。

建议读者参考 Ruelle(1969),Dobrushin(1968),Lanford,Ruelle(1969)和 Gallavotti et al. (1999)。

维里定理和原子尺度

很长时间以来,人们一直怀疑"仅改变边界条件"会产生如宏观不同态一样的剧烈变化(即以上一节意义上定义的相变)。最初的根据是考虑热力学极限下非常有规则的解析函数,例如 $N^{-1}\log Z^c(\beta,N,V)$(是 $\beta,v=V/N$ 的函数),在 $\Omega\to\infty$ 的极限条件下出现奇点,就像在范德瓦耳斯理论的气液相变中出现的不连续产物(相应于式[16]中最大值出现的平台以及接下来的几个单相共存的情况)。

考虑由质量为 m 的 N 个全同粒子组成的真实气体,这些粒子位于一个体积为 V 的容器 Ω 中。假设第 i 个粒子上的作用力为 $\boldsymbol{f}_i$;在运动方程 $m\ddot{\boldsymbol{q}}_i=\boldsymbol{f}_i$ 的两边同时乘以 $-(1/2)\boldsymbol{q}_i$ 并对所有的 i 求和:即

$$-\frac{1}{2}\sum_i^N m\boldsymbol{q}_i\cdot\ddot{\boldsymbol{q}}_i=-\frac{1}{2}\sum_i^N\boldsymbol{q}_i\cdot\boldsymbol{f}_i\overset{\text{def}}{=}\frac{1}{2}C(\boldsymbol{q})$$

这里 $C(\boldsymbol{q})$定义为位形 $\boldsymbol{q}$ 中的**维里力**。注意 $C(\boldsymbol{q})$不是平移不变量,这是因为存在由容器壁产生的作用力。

把作用力 $\boldsymbol{f}_i$ 写成粒子内部相互作用力和外部作用力(容器壁产生的)的和,那么维里力 C 也可以很自然地表示成内部维里力 C_{int}(平移不变量)和外部维里力 C_{ext} 之和。

在维里定义的两边同时除以 τ 并在时间间隔$[0,\tau]$上做积分,我们发现在 $\tau\to+\infty$,也就是说,当 $\tau\to\infty$ 时,物理量足够小,有

$$\langle K\rangle=\frac{1}{2}\langle C\rangle\text{ 和}\langle C_{\text{ext}}\rangle=3pV$$

这里 p 是压强,V 是体积。因此有

$$\langle K\rangle=\frac{3}{2}pV+\frac{1}{2}\langle C_{\text{int}}\rangle$$

或

$$\frac{1}{\beta}=pv+\frac{\langle C_{\text{int}}\rangle}{3N}\qquad[24]$$

方程[24]就是**克劳斯维里定理**,在没有内部相互作用的情况下,它变成 $\beta pv=1$,也就是理想气体方程。

如果 $\boldsymbol{f}_{j\to i}=-\partial_{\boldsymbol{q}_i}\varphi(\boldsymbol{q}_i-\boldsymbol{q}_j)$,则内部维里力 C_{int} 可以写成如下形式:

$$\begin{aligned}C_{\text{int}}&=-\sum_{i=1}^N\sum_{i\neq j}\boldsymbol{f}_{j\to i}\cdot\boldsymbol{q}_i\\&\equiv-\sum_{i<j}\partial_{\boldsymbol{q}_i}\varphi(\boldsymbol{q}_i-\boldsymbol{q}_j)\cdot(\boldsymbol{q}_i-\boldsymbol{q}_j)\end{aligned}$$

这表明内部的排斥力对维里力的贡献是负的,而吸引力的贡献是正的。C_{int} 的平均值可以很方便地利用正则分布计算出来。范德瓦耳斯首次将维里定理应用在一个对理想气体定律的修正计算上。简单忽略密度的三次方项并将式[23]中的关联函数取近似 $\rho(\boldsymbol{q}_1,\boldsymbol{q}_2)=\rho^2\mathrm{e}^{-\beta\varphi}(\boldsymbol{q}_1,\boldsymbol{q}_2)$,就得到

$$\frac{1}{2}\langle C_{\text{int}}\rangle = V\frac{3}{2\beta}\rho^2 I(\beta) + VO(\rho\kappa^3) \qquad [25]$$

这里

$$I(\beta) = \frac{1}{2}\int(\mathrm{e}^{-\beta\varphi(q)} - 1)\mathrm{d}^3\boldsymbol{q},$$

状态方程[24]变成

$$pv + \frac{I(\beta)}{\beta v} + O(v^{-2}) = \beta^{-1}$$

为了说明的目的,I 值的计算可以在(经典的纳纳德-琼斯势)

$$\varphi(r) = 4\varepsilon\left(\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^{6}\right)$$

($\varepsilon, r_0 > 0$)且高温(小 β)近似的情况下进行,其结果是

$$I \approx -(b - \beta a)$$

$$b = 4v_0, a = \frac{32}{3}\varepsilon v_0, v_0 = \frac{4\pi}{3}\left(\frac{r_0}{2}\right)^3$$

因此有

$$pv + \frac{a}{v} - \frac{b}{\beta v} = \frac{1}{\beta} + O\left(\frac{1}{\beta v^2}\right)$$

$$\left(p + \frac{a}{v^2}\right)v = \left(a + \frac{b}{v}\right)\frac{1}{\beta} = \frac{1}{1 - b/v}\,\frac{1}{\beta} + O\left(\frac{1}{\beta v^2}\right)$$

或

$$\left(p + \frac{a}{v^2}\right)(v - b)\beta = 1 + O(v^{-2}) \qquad [26]$$

给出了 $\beta\varepsilon \ll 1$ 时的状态方程。方程[26]可以跟人们所熟知的经验式的范德瓦耳斯状态方程:

$$\beta\left(p + \frac{a}{v^2}\right)(v - b) = 1$$

或

$$(p + An^2/V^2)(V - nB) = nRT \qquad [27]$$

做比较。这里,如果 N_A 是阿伏加德罗常数,$A = aN_A^2$,$B = bN_A$,$R = k_B N_A$,$n = N/N_A$。这表明,可以通过测量稀薄气体的实验值对波伊耳-马略特定律 $\beta pv = 1$ 的偏离来确定微观势 φ 中的参数值 ε 和 r_0:$\varepsilon = 3a/8b = 3A/8BN_A$,$r_0 = (3b/2\pi)^{1/3} = (3B/2\pi N_A)^{1/3}$。

最后值得一提的是,维里定理原则上以一种直接而简单的方式给出了状态方程的准确修正,这个修正是内部作用的维里力的时间平均。由于内部作用的维里力可以简单地由随时间变化的粒子位置计算出来,这个定理提供了一个用数值模拟处理状态方程的方法。事实上,这个方法已经在很多数值计算中使用,在这里,式[24]起到了关键作用。

更多的详细资料,读者可参考 Gallavotti(1999)的文献。

范德瓦耳斯理论

范德瓦耳斯方程[27]的形式常被经验性地推广到超越其适用条件(低密高温)的区域,其中 A, B 被看做唯象参数,由测量任意一组 p, V, T 的实验值确定。测得的 A, B 作

为 v,T 的函数值,通常不会变化很多。如果不考虑这个小小的变化,式[27]给出的预言往往能够很好的符合实验,不过随着实验精度的逐年提高,这个公式的严重不足才显示出来。

由式[27]得到的一系列结果都是很吸引人的。比如,图 1 说明,如果温度足够低,就不会出现 p 随 v 的单调非增变化。由此可以定义一个临界温度 T_c 作为最大值,在这个温度之下,p 作为 v 的函数不是单调下降的;临界体积 V_c 是当 $T=T_c$ 时,v 在水平拐点处的体积。

当 $T<T_c$ 时,范德瓦耳斯对状态方程的解释是:函数 $p(v)$ 描述了亚稳态,而实际的平衡态遵循单调的对 v 的依赖关系,$p(v)$ 在特殊体积共存区域是一条水平线段。画 p 的水平线时(见图 1),它的精确值既可以由实验确定,也可以在理论上由一个简单的原则预言,这个简单的原则就是,画出的水平线与等温线围成的两个回路面积相等。

这就是麦克斯韦等面积法则:它能够成立的条件是假设等温线以及端点在等温线上的水平线构造了一个回路(见图 1),这个回路表示存在一系列可能的宏观平衡态(对应于水平线的那些平衡态)或者由弯曲部分表征的具有足够长时这个循环中所做的功(如 $\oint p\mathrm{d}v$)等于回路所包围的带正负号的面积,所以这个面积等于零,这就是等面积法则。这样的讨论值得怀疑,至少因为那些 p 随 v 增加的中间态是否能在实验上找到,或者只存在理论上的可能性,这些并不清楚。

式[27]有一个惊人的预言,气体经历了一个气—液相变,这个相变有临界点,临界温度 T_c、临界体积 V_c 和临界压强 p_c 可以通过式[27]计算出来:$RT_c=8A/27B$,$V_c=3B(n=1)$。

同时,上面的预言的有趣之处在于其给出了一个临界参数和微观相互作用常数之间的简单关系,那就是 $\varepsilon\approx k_BT_c$ 和 $r_0\approx(V_c/N_A)^{1/3}$,如果以 Lennard-Jones 势做为相互作用势($\varphi=4\varepsilon((r_0/|q|)^{12}-(r_0/|q|^6)$,参见上一节),这个关系能准确地表述为 $\varepsilon=81k_BT_c/64$ 和 $r_0=(V_c/2\pi N_A)^{1/3}$。

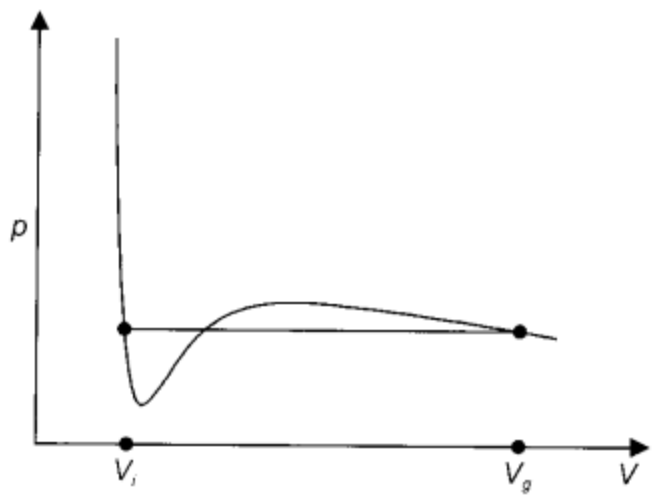

图 1 温度 $T<T_c$ 时的范德瓦耳斯状态方程,这里压强不是单调的。横线表示"麦克斯韦等面积法则"。

然而,式[27]不能被轻易地认可,不仅因为得到它时所采用的近似(本质上是在状态方程中忽略了 $O(v^{-1})$),更主要是因为 p 必须是 v 的单调函数(参见式[19]下面的评注),但是正如上面所提到那样,对于 $T<T_c$,p 不再是 v 的单调函数了。

由麦克斯韦等面积法则,范德瓦耳斯方程得到了改进,它能够给出以下关系:

$$\begin{aligned}&(p-p_c)\propto(v-v_c)^{\delta},\delta=3,T=T_c\\&(v_g-v_l)\propto(T_c-T)^{\beta},\beta=1/2(\text{当 }T\to T_c^{-}\text{ 时})\end{aligned}\qquad[28]$$

这个关系与 20 世纪的实验得到的结果存在尖锐的矛盾。对于最简单的情况,人们发现 $\delta\approx5$,$\beta\approx1/3$。

最后,对状态方程[27]的盲目信任站不住脚了,这是因为如果空间维数是 $d=2$ 或

$d=1$,分析没有什么改变;但是对于 $d=1$,很容易证明对于在无穷远处衰减很快的相互作用系统不存在相变(见下一节)。

事实上,现在人们知道范德瓦耳斯方程只在限定的情况下才是严格的,它要求粒子的相互作用势有一个硬核(或近程强排斥)且长程光滑。更准确地说,假如作用势在硬核半径 $r_0>0$ 以外是吸引势(非负),且有 $\gamma^d\varphi_1(\gamma^{-1}|\boldsymbol{q}|)\leqslant 0$ 的形式,我们可以定义 $P_0(v)$(依赖于 β)为 β 与硬核系统压强的乘积,这个硬核系统无任何吸引势尾(当 $d=1$ 时,$P_0(v)(v-b)=1$,$b=r_0$,其他情况下 $P_0(v)$ 没有确定的形式),并且让

$$a=\frac{1}{2}\int_{|\boldsymbol{q}|<r_0}|\varphi_1(\boldsymbol{q})|\,d\boldsymbol{q}$$

如果当 $\gamma>0$ 时 $p(\beta,v;\gamma)$ 是压强,那么可以证明

$$\beta p(\beta,v)\overset{\text{def}}{=}\lim_{\gamma\to 0}\beta p(\beta,v;\gamma)=\left[-\frac{\beta a}{v^2}+P_0(v)\right]_{\text{麦克斯韦法则}} \qquad [29]$$

其中脚标表示 $p(\beta,v)$ 随 v 的变化图是由方括号中的函数在麦克斯韦等面积法则的约束下得到的,麦克斯韦等面积法则在上面讲范德瓦耳斯方程的时候提到。当 $d=1$ 时,方程[29]可以严格地回到范德瓦耳斯方程;当 $d>1$ 时,它是一个能描述同种临界行为的方程(即使 $P_0(v)$ 不能严格计算)。

更多细节,读者可以参考 Lebowitz,Penrose(1979)和 Gallavotti(1999)等人的文献。

$d=1$: 无相变

统计物理中最著名的一个不存在定理就是在一维短程相互作用粒子系统中没有相变(参考下一节),除非考虑热力学零温这种多少有些非物理的情况。在"最近邻硬核相互作用"情况下,这一定理很好验证。设硬核半径是 r_0,相互作用势为当 $r\leqslant r_0$ 时,$\varphi(r)=+\infty$,并假设当 γ[①]$\geqslant 2r_0$ 时,$\varphi(r)\equiv 0$。在这种情况下,热力学函数可以精确计算并且是解析的:因此状态方程不会有任何相变平台。这是 van Hove 定理的一种特殊情况,该定理证明了在相互作用超越最近邻且在无穷大处迅速衰减时状态方程的平滑性。

如果采用基于热力学极限对不同边界条件的敏感性的相变定义的话,则更普遍的,概念上也更简单的论述表明,在一维系统中,一个处于参考粒子(比如处于原点 O)左边的构形为 Q 的粒子系统和处于参考粒子右边的构形为 Q'(满足关系 $Q\cup O\cup Q'$,与硬核势一致)的粒子系统之间的相互作用势如果一致有下界,则该系统是不会有任何相变的。一个数学定理证明当边界趋于无穷大时,边界条件的影响消失。在不考虑边界条件影响的情况下,我们也可以说在一维情况下没有长程序。

如果空间维数大于等于 2 的时候,该论述不成立。这时,即使相互作用是短程的,由边界分开的两个空间区域之间的相互作用能是和边界区域的大小同一个量级。因此,对任意两个构形,不能通过其忽略另外一半空间的几率的直乘得到它们两个在半空间的几率的上界和下界。因为这样的界随分离表面指数增加,在表面增大时会趋于无穷。这就意味着,至少对普遍的情况,我们不能认为两个半空间的构形是独立分布的。

解析上,一个加在势能上的条件可以充分保证原点左右两边构形之间的能量有下界,

① 原文为 f,似有误——译者注。

如果 $d=1$,该条件可简单表达为

$$\int_{\gamma}^{\infty} r\,|\varphi(r)|\,\mathrm{d}r<+\infty \quad r'>r_0$$

因此,如果要使 $d=1$ 情况下发生相变,需要一个"如此长程"的势能,以至它的首项就发散。反例可以证明如果该条件不需满足,即使在 $d=1$ 系统中也可以发生相变。

上述结果也适用于离散系统,如本文后面会考虑到的格子气与格点自旋系统。

更多论述,读者可参考文献 Landau, Lifschitz (1967), Dyson (1969), Gallavotti (1999),以及 Gallavotti et al. (2004)等。

连续对称性:"无 $d=2$ 晶体"定理

第二种情况,有很好对称性的系统可以排除相变可能或至少某些种类的相变可能,这里的对称是指一组作用在构形上的变换,使其中每一个构形变为至少在一种(如周期或开放)边界条件下,与之有相同能量的另一种构形。

如果对应的变换群是连续群,就说此对称是"连续"的。比如,在一个具有周期性边界条件的容器 Ω 中的连续系统具有平移对称性。一个"具有太多对称性"的系统有时不会发生相变。比如,在一个具有周期性边界条件的容器 Ω 中,气体的连续平移对称性在维数 $d=2$ 时足以排除任何晶体化的可能。

这个问题是一个证明的范式,而这个证明可以用来推断具有连续对称性系统中许多相变的缺失,为了讨论该问题,考虑平移对称性和一个势能,除了满足式[14]中所引的普遍性质(并采用其中的符号)外,对某些 $\bar{B}$,在 $r_0<|\boldsymbol{q}|\leqslant R$ 范围内,需进一步满足 $|\boldsymbol{q}|^2|\partial_{ij}^2\varphi(\boldsymbol{q})|<\bar{B}|d|^{-(d+\epsilon_0)}$,其中 $\epsilon_0>0$。这个条件并不十分难满足(并且与硬心势兼容)。

为简单起见,考虑一个空间正方晶格中的"理想晶体",恰好置于边长为 L,具有周期性边界条件的容器 Ω 中,则粒子数为 $N=(L/a)^d$,密度是 a^{-d},如果相互作用 φ 是硬核势,则该密度比密堆晶格的密度小。粒子的概率分布是非常平凡的:

$$\bar{\mu}=\sum_{p}\prod_{n}\delta(\mathbf{q}_{p(\mathbf{n})}-a\mathbf{n})\,\frac{d\boldsymbol{Q}}{N!}$$

求和遍及置换 $\boldsymbol{m}\to p(\boldsymbol{m})$,格点 $\boldsymbol{m}$ 满足 $\boldsymbol{m}\in\Omega,\boldsymbol{m}\in\mathbb{Z}^d$, $0<m_i\leqslant La^{-1}$。$\boldsymbol{q}$ 处的密度为

$$\hat{\rho}(\boldsymbol{q})=\sum_{\mathbf{n}}\delta(\boldsymbol{q}-a\boldsymbol{n})\equiv\left\langle\sum_{j=1}^{N}\delta(\boldsymbol{q}-\boldsymbol{q}_i)\right\rangle$$

其傅里叶变换正比于

$$\rho(k)\overset{\text{def}}{=}\frac{1}{N}\left\langle\sum_{j}e^{-i\boldsymbol{k}\cdot\mathbf{q}_j}\right\rangle,\boldsymbol{k}=\frac{2\pi}{L}\boldsymbol{n},\boldsymbol{n}\in\mathbb{Z}^d$$

这里对于所有满足 $\boldsymbol{K}=(2\pi/a)\boldsymbol{n}$ 的 $\boldsymbol{k}$,$\rho(\boldsymbol{k})$ 的值是 1,其余的情况是 $(1/N)O(\max_{\tau=1,2}|\mathrm{e}^{ik_\tau a}-1|^{-2})$。在有相互作用的情况下,必需有,在一个晶体态中,$\rho(\boldsymbol{k})$ 在 $\boldsymbol{K}$ 附近有最大值;但 $\rho(\boldsymbol{k})$ 的值依赖于边界条件。

因为系统具有平移不变性,一个晶体态(定义为分布接近 $\bar{\mu}$ 的态),即 $\hat{\rho}(q)$ 恰在理想晶格的格点 $\boldsymbol{q}=\boldsymbol{n}a$ 上取最大值,在周期性边界条件下并不能实现,即使系统的状态是类晶的,为了实现这样的晶体态,相互作用中需要引入对称破缺项。

实现的方法有多种,例如改变边界条件。这个选择意味着要讨论边界条件对 $\rho(\boldsymbol{k})$ 的

峰值有多大影响:比如,边界条件不会与选好的另一个条件(可能与原条件对应不同的倒格矢 $\boldsymbol{K}$)产生不同的周期,这并不明显。因此我们选择想像有个对应势能 $\varepsilon W(q)$ 的弱外作用导致对称更容易破缺到占据理想晶格的格点周围区域(对应所选择的晶体态下粒子的平均位置)。Mermin 定理表明,没有平衡态对应与 $\bar{\mu}$ 很"接近"的分布,即其峰值处在 δ 函数处。下面的内容是这个定理的再现。

取 $W(\boldsymbol{q})=\sum_{\boldsymbol{na}\in\Omega}\chi(\boldsymbol{q}-\boldsymbol{na})$,其中 $\chi(\boldsymbol{q})\leqslant 0$ 是光滑的,且在除格点附近的极小区域外均为零,在格点处函数值下降到某个负的极小值并保持旋转对称性。势能 W 是沿着晶格矢量平移不变的。如果选择合适的边界条件和 εW,密度 $\tilde{\rho}_\varepsilon(q)$ 将是周期函数,周期为 a,故 $\rho_\varepsilon(\boldsymbol{k})$ 有可能在 $N\to\infty$ 时极限不为零,$\boldsymbol{k}$ 是一个倒格矢 $\boldsymbol{K}=(2\pi/a)\boldsymbol{n}$ 时例外。如果势能为 $\varphi+\varepsilon W$ 并且存在一个晶体态,其中粒子有较大几率出现在格点 $\boldsymbol{na}$ 附近,可以预想对小的 $\varepsilon>0$,系统将处在这样一个态,其密度的傅里叶变换 $\rho_\varepsilon(k)$ 对倒点阵中的矢量 $\boldsymbol{K}\neq 0$ 有

$$\lim_{\varepsilon\to 0}\lim_{N\to\infty}|\rho_\varepsilon(\boldsymbol{K})|=r>0 \qquad [30]$$

就是说,要求在 $\varepsilon\to 0$ 的过程中,密度的傅里叶变换对某个 $\boldsymbol{K}\neq 0$ 总有一个峰值。注意如果 $\boldsymbol{k}$ 不是在倒点阵,有 $\rho_\varepsilon(\boldsymbol{k})\xrightarrow[N\to\infty]{}0$,该式有上界

$$\frac{1}{N}O\left(\max_{j=1,2}\left|\mathrm{e}^{\mathrm{i}k_j a}-1\right|^{-2}\right)$$

因为 $(1/N)\tilde{\rho}_\varepsilon$ 是周期的且对 $\boldsymbol{q}$ 的积分等于 1,所以式[30]的不可能就等同于排除了晶体的存在。其他的判据如,考虑一个晶格不是简单的立方晶体,类似的处理会得出同样的结果。但是数学上并没有排除(尽管不大可能)在更弱的定义下,晶体态在二维的可能性。

仍然在目前的势能假设下,考虑箱子 Ω,边长为 a 的整数倍(故有 $N=(La^{-1})^d$),考虑正则分布、周期性边界条件、参数 (β,ρ)、$\rho=a^{-3}$、相互作用势 $\varphi+\varepsilon W$,下面的不等式成立。当相互作用势是硬核势时,当然需要进一步假设晶格 $\mathbf{n}a$ 不是密堆结构。因此,对合适的 $B_0,B,B_1,B_2>0$,不依赖于 N、ε,对满足 $\kappa<\pi/a$,且对所有的 Ω(如果 $\boldsymbol{K}=0$)有

$$\frac{1}{N}\left\langle\left|\sum_{j=1}^{N}\mathrm{e}^{-i(\kappa+\mathbf{K})\cdot\boldsymbol{q}_j}\right|^2\right\rangle\geqslant B\frac{(\rho_\varepsilon(\boldsymbol{K})+\rho_\varepsilon(\boldsymbol{K}+2\kappa))^2}{B_1\kappa^2+\varepsilon B_2}$$

$$\frac{1}{N}\sum^{\kappa}\gamma(\kappa)\frac{\mathrm{d}\kappa}{N}\left\langle\left|\sum_{j=1}^{N}e^{-i(\kappa+\mathbf{K})}\cdot\boldsymbol{q}_j\right|^2\right\rangle\leqslant B_0<\infty \qquad [31]$$

其中求平均是在周期性边界条件和对称破缺势 $\varepsilon\boldsymbol{W}(\boldsymbol{q})$ 下对正则分布 (β,ρ) 进行的;$\gamma(\boldsymbol{k})\geqslant 0$ 是任意光滑函数,当 $2|\kappa|\geqslant\delta$、$\delta<2\pi/a$ 时函数为零。B_0 的值依赖于 γ。不满足式[31]的情况参见附录三。

将式[31]的第一个方程两边同时乘以 $N^{-1}\gamma(\kappa)$ 并对 κ 求和,由式[30]中的晶体性条件有

$$B_0\geqslant Br^2\,a^d\int_{|\kappa|<\delta}\frac{\gamma(\kappa)\mathrm{d}\kappa}{\kappa^2B_1+\varepsilon B_2}$$

对 $d=1,2$,积分分别按照 $\varepsilon^{-1/2}$ 或 $\lg\varepsilon^{-1}$ 发散,故而 $|\rho_\varepsilon(\boldsymbol{K})|\xrightarrow[\varepsilon\to 0]{}r=0$:晶体性的判据[30]对 $d=1,2$ 不满足。

上面的不等式是更广义的红外不等式的一个推广,而红外不等式源于博戈留波夫不等式(见附录三),博戈留波夫不等式可以用来证明当包围其空间的维数是 $d=2$ 时,在合适的(如周期性)边界条件下,如果有限体积具有连续对称性,则某些有序相不存在。这种排除现象,更准确得地说是热力学极限下,有限体积中表现出的低于连续对称性的对称性的平衡态不存在。

普遍来说,在一定的边界条件下存在一些热力学平衡态,其对称性低于有限体积下系统的对称性,称作"自发对称破缺"。它实际上是对边界条件变换不稳定性的另一个表现,因此自发对称破缺对应相变。对一大类系统而言,红外不等式暗示自发对称破缺的缺失:在大多数一维或二维系统中,连续对称性是不会自动破缺的。

$d\leqslant 2$ 对红外定理用来排除相变可能的普遍应用是很强的一个限制,更准确地讲,系统可以分为几类,每一类都有一个临界维数,低于这个临界维数时太多的对称性导致相变(或某些种类的相变)的缺失。

应该强调,在临界维度,对称破缺的禁止通常很弱,需要极大的容器来破坏实现对称破缺的微小效应(边界条件或非常弱的场)。例如在刚刚讨论的晶体化问题中,傅里叶变换的峰值只有量级 $O(1/\sqrt{\lg\varepsilon^{-1}})$。因此,从实际问题的角度出发,即使在很大的容器中,某种序的存在仍然是可能的。

读者参考文献 Mermin(1968),Hohenberg(1969)和 Ruelle(1969)。

高温和低密度

有这样一类不发生相变的系统。这类系统在高温、低密度状态有稳定且缓和的相互作用 φ(例如,那些满足式[14]的相互作用)。这一性质可以通过将状态方程以 (β,ρ) 为变量在(0,0)附近展开而得到。

一种简单的方法(Mayer 级数)可以得到维里展开的各项系数:

$$\beta p(\beta,\rho)=\rho+\sum_{k=2}^{\infty}c_k(\beta)\rho^k$$

它的缺点就是第 k 阶展开系数 $c_k(\beta)$ 是许多项的和(项的个数增加的速度比按照 k 的 e 指数的形式增加还快),而且如果 β 足够小,将这些项的和以 k 的 e 指数形式组合表示并不容易(尽管是可能的)。一种更有效的方法可以很快得到想要的结果。记 $\Phi(q_1,\cdots,q_n)=\sum_{i<j}\varphi(q_i-q_j)$,以 β,λ 为巨正则分布的参数,按照关联函数(空间或者构形)的定义

$$\rho_\Omega(q_1,\cdots,q_n)\equiv\frac{1}{Z^{gc}(\beta,\lambda,V)}\sum_{m=0}^{\infty}Z^{n+m}\times\int_\Omega \mathrm{e}^{-\beta\Phi(q_1,\cdots,q_n,y_1,\cdots,y_m)}\frac{\mathrm{d}y_1\cdots\mathrm{d}y_m}{m!}\quad[32]$$

这是发现有粒子处于体积元 $\mathrm{d}q_1\cdots\mathrm{d}q_m$ 内,而不考虑其动量是多少的概率(不考虑其他粒子的位置),而且 $z=\mathrm{e}^{\beta\lambda}(\sqrt{2\pi m\beta^{-1}b^{-2}})^d$ 是配分函数对动量积分所得到项,称之为活动度:具有密度的量纲(比较式[23])。

为了简单,假设势能是半径为 R 的硬核势,有一个粒子固定在位置 q_1,而其他粒子处于 $(q_2,\cdots,q_m)$,并且要求 $|q_i-q_j|>R$ 的内能 $\Phi_{q_1}(q_2,\cdots,q_m))$ 的下界为 $-B$,$B\geqslant 0$(与式[14]中的 B 有关,但并不相等)。函数 ρ_Ω 被看作是一个两个粒子,…的位置函数的序列。$\rho_\Omega=\{\rho_\Omega(q_1,\cdots,q_n)\}_{n=1}^{\infty}$,当 $q_j\notin\Omega$ 时此式为零。那么,有

$$\rho_\Omega(q_1,\cdots,q_n) = z\delta_{n,1}\chi_\Omega(q_1) + K_{\rho_\Omega}(q_1,\cdots,q_n) \qquad [33a]$$

这里,

$$K_{\rho_\Omega}(q_1,\cdots,q_n) \equiv \mathrm{e}^{-\beta\Phi_{q_1}(q_2,\cdots,q_n)}(\rho_\Omega(q_2,\cdots,q_n)\delta_{n>1} + \sum_{s=1}^{\infty}\int_\Omega \frac{\mathrm{d}y_1\cdots\mathrm{d}y_s}{s!}\prod_{k=1}^{s}(\mathrm{e}^{-\beta\varphi(q_1-y_k)}-1)\times\rho_\Omega(q_1,\cdots,q_n,y_1,\cdots y_s) \qquad [33b]$$

在这里,$\delta_{n,1}$,$\delta_{n>1}$是克罗内克函数,$\chi_\Omega(q)$是 Ω 的指示函数。等式[33]被称作 Kirkwood-Salzburg 方程。K 与 Ω 无关,但是积分区域是 Ω。

记 α_Ω 为一系列函数 $\alpha_\Omega(q_1,\cdots,q_n)\equiv 0$,(如果 $n\neq 1$)且 $\alpha_\Omega(q)=z\chi_\Omega(q)$,我们就得到一个递归的展开式

$$\rho_\Omega = z\alpha_\Omega + z^2K\alpha_\Omega + z^3K^2\alpha_\Omega + z^4K^3\alpha_\Omega + \cdots \qquad [34]$$

级数是收敛的,关联函数可以由此得到。由不等式

$$|K^p\alpha_\Omega(q_1,\cdots,q_n)| \leqslant \mathrm{e}^{(2\beta B+1)p}\left(\int|\mathrm{e}^{-\beta\varphi(q)}-1|\,\mathrm{d}q\right)^p = \mathrm{e}^{(2\beta B+1)pr}(\beta)^{3p} \qquad [35]$$

可以知道 Mayer 展开在 $|z|<\mathrm{e}^{-(2\beta B+1)p_r}(\beta)^{-3}$ 时是收敛的。当 $\Omega\to\infty$ 时是一致收敛的,而且当 $\rho(q_1,\cdots,q_n)\equiv 0(n\neq 1)$ 且 $\alpha(q_1)\equiv 1$ 时,$(K^p)\rho_\Omega(q_1,\cdots,q_n)$在固定点 $q_1,\cdots,q_n$ 处,当 $V\to\infty$ 时的极限是$(K^p\alpha)(q_1,\cdots,q_n)$。这是因为 K 中包含$(\mathrm{e}^{-\beta\varphi(q_1-y_k)}-1)$因子,这一项衰减的非常快,或者如果 φ 的是有限值,这一项最终要变为零,而且$(K^p\alpha)(q_1,\cdots,q_n)$具有变换不变性。

所以,如果$|z|<\mathrm{e}^{-(2\beta B+1)p_r}(\beta)^{-3}$,那么当 $\Omega\to\infty$ 时,关联函数是存在的,而且可以通过关于 z 的级数展开得到;关联函数在热力学极限下具有变换不变性。

特别的,单点关联函数 ρ,$\rho=z(1+O(zr(\beta)^3))$,作为 z 的最低级展开,当密度和活动度很小时,它们可以看作是相等的。另外,$\beta p_\Omega=\frac{1}{V}\lg Z^{\mathrm{gr}}(\beta,\lambda,V)$可以通过

$$z\partial_z\beta p_\Omega = \frac{1}{V}\int\rho_\Omega(q)\,\mathrm{d}q$$

得到

$$p(\beta,z) = \lim_{V\to+\infty}\frac{1}{V}\lg Z^{\mathrm{gr}}(\beta,\lambda,V) = \int_0^z\rho(\beta,z')\,\frac{\mathrm{d}z'}{z'} \qquad [36]$$

密度 ρ 对 z 是解析的,而且当 z 很小时,$\rho\approx z$,而且巨正则系统的压强对密度也是解析的,当密度很小时,$\beta p=\rho(1+O(\rho^2))$。换句话说,状态方程的最低阶展开就是理想气体的状态方程。所有的热力学量都是温度和密度的解析函数。这个系统实质上就是自由气体,没有相变发生。而且,强烈依赖于有固定外界粒子的边界条件的相变也不会发生。这些结果可以通过额外的推理由 Kirkwood-Salzburg 等式得到。

更多的细节,读者可以参考 Ruelle(1969)和 Gallavotti(1969)的文章。

格点模型

对于均匀气体在两体作用势下,是否存在相变的问题仍然是很活跃的一个领域。因此,研究简单系统的相变行为是很有意义的。模型虽然简单,但是并非不重要,有些还是

非常有趣的。

最简单的模型就是所谓的格点模型,在这个模型里粒子被限制在格点上,用通常的话来说,粒子不能运动(但是可以在格点之间跳跃)。所以我们不用考虑动量变量。

内能只包括势能,而且系综被定义为粒子位形的位置坐标概率分布函数的集合。通常势能在无穷远处快速衰减,而且有一个硬核以防止两个或更多的粒子占据同一个位置。例如,具有相互作用 φ 的格子气,格子的总体积为 $|\Omega| = V = L^d$,格点间相距为 $a>0$。由不同的格点所组成的构型 X 的势能被定义为

$$H(X) = -\sum_{(x,y)\in X}\varphi(x-y) \qquad [37]$$

这里子集 $X\subset\Omega$,求和是对 X 构形里所有不同的点进行的。正则和巨正则系综的分布函数以 (β,ρ),$[\rho=N/V]$ 或者 (β,λ) 为参数。则 X 构形出现的几率为

$$p_{\beta,\rho}(X) = \frac{e^{-\beta H(X)}}{Z_p^c(B,N,\Omega)}\delta_{|X|,N} \qquad [38a]$$

或者

$$p_{\beta,\lambda}(X) = \frac{e^{\beta|X|}e^{-\beta H(X)}}{Z_p^{gc}(\beta,\lambda,\Omega)} \qquad [38b]$$

几率已经被归一化,归一化因子称作正则和巨正则配分函数;下标 p 代表粒子。

格子气的每一个格点上最多只有一个粒子,这和一个格点上有一个自旋的模型非常相似。自旋模型非常有名而且有很强的实用价值(当初是为研究磁性材料的性质而提出的)。简单说,一个格点被粒子占据则记为自旋向上或者+,没有粒子占据则记为自旋向下或记为−。如果记 $\sigma=\{\sigma_x\}_{x\in\Omega}$ 为自旋的构形,格点间相互作用为 φ,外磁场为 h,则系统的哈密顿量为

$$H(\sigma) = \sum_{(x,y)\in X}\varphi(x-y)\sigma_x\sigma_y - h\sum_x\sigma_x \qquad [39]$$

求和是对 Ω 内所有不同的点进行。如果 $\varphi(x-y)\equiv J_{xy}\geqslant 0$,这个模型就称为铁磁伊辛模型。对于连续的系统,假设 φ 的作用很有限,除非明确另外说明,对于某个 R,当 $|x|>R$ 时,$\varphi(x)=0$。

在正方体体 Ω 内,分别具有参数 (β,m) 或者 (β,h) 的正则和巨正则系综,由加或不加限制条件 $\Sigma_{x\in\Omega}\sigma_x = M = mV$ 的自旋构型 $\sigma=\{\sigma_x\}_{x\in\Omega}$ 的几率分布分别是

$$p_{\beta,m}(\sigma) = \frac{\exp(-\beta\Sigma_{(x,y)}\varphi(x-y)\sigma_x\sigma_y)}{Z_s^c(\beta,M,\Omega)}$$

$$p_{\beta,h}(\sigma) = \frac{\exp(-\beta h\Sigma\sigma_x - \beta\Sigma_{(x,y)}\varphi(x-y)\sigma_x\sigma_y)}{Z_s^{gc}(\beta,h,\Omega)} \qquad [40]$$

来定义。这里的分母是归一化因子,仍分别被称作正则和巨正则系综的配分函数。按照以前研究连续系统的方法,具有外部固定粒子构形的正则和巨正则系综可以一起被定义为具有外部固定自旋的构形的系综;下标 s 代表自旋。

对于格子气的每一个构形 $X\subset\Omega$,如果 $x\in X$ 则 $n_x=1$,如果 $x\notin X$ 则 $n_x=0$。那么变换关系 $\sigma_x=2n_x-1$ 就建立了从格子气模型到自旋模型之间的联系。相应的格子气模型的相互作用式 $\varphi(x-y)$ 对应着自旋模型的相互作用式 $\frac{1}{4}\varphi(x-y)$,格子气模型的化学势 λ

对应着自旋模型的外磁场强度 h,$h=\frac{1}{2}(\lambda+\Sigma_{x\neq 0}\varphi(x))$。

边界条件之间的变换也是很自然的,在格子气中格点被占据的对应着自旋模型中外部格点为+。格子气和自旋模型之间的转换就不再多费笔墨了。

在格子气模型中,经常考虑的是周期性边界条件(在 Ω 以外没有格点)。在格子气和自旋模型中(连续系统也是如此),周期和半周期边界条件(在一个或多个方向采用周期性边界条件,在其他方向有固定外部粒子或自旋,或者空位)经常用到。

利用和附录二类似的方法,我们可以证明配分函数在热力学极限下是存在的:

$$\begin{aligned}
-\beta f(\beta,v) &= \lim_{\substack{\Omega\to\infty \\ V/N=v}} \frac{1}{N}\lg Z_p^c(\beta,N,\Omega) \\
\beta p(\beta,\lambda) &= \lim_{\Omega\to\infty} \frac{1}{V}\lg Z_s^c(\beta,\lambda,\Omega) \\
-\beta g(\beta,m) &= \lim_{\substack{\Omega\to\infty \\ M/V\to m}} \frac{1}{V}\lg Z_s^{gc}(\beta,M,\Omega) \\
\beta f(\beta,h) &= \lim_{\Omega\to\infty} \frac{1}{V}\lg Z_s^{gc}(\beta,\lambda,\Omega)
\end{aligned} \qquad [41]$$

它们的凹凸性和连续性与连续系统是一样的。在格子气中 f,p 被定义为自由能和压强。在自旋模型中 $f(\beta,\rho)$ 被解释为磁自由能,然而 $g(\beta,m)$ 在自旋系统里没有一个特殊的名称。像在连续系统中一样,定义无限大体积的平衡态是有帮助的。

定义 一个具有参数 (β,h) 或 (β,m) 之无限大体积系统的状态是一系列平均值 $F\to\langle F\rangle$。在有限体积 Ω_n,给定参数 (β,h) 或 (β,m),或 (u,v),具有固定外部自旋或空位的边界条件,由正则或巨正则系综分布定义平均值 $\langle F\rangle_{\Omega_n}$,然后在 $\Omega_n\to\infty$ 极限下,所有局部观测量 F 的极限都同时成立。

我们逐字采用"相变和边界条件"一节中的定义。如果 $\sigma_X=\Pi_j\sigma_{\xi_j}$,那么对 $X=(\xi_1,\cdots,\xi_n)$ 定义关联函数 $\langle\sigma_X\rangle$ 是有意义的。例如,我们有 $\rho(\xi_1,\xi_2)\overset{\text{def}}{=}\langle\sigma_{\xi_1}\sigma_{\xi_2}\rangle$,可以将一个纯相定义为一个无限大体积态,以至于

$$\lim_{\xi\to\infty}[\langle\sigma_X\sigma_{Y+\xi}\rangle-\langle\sigma_X\rangle\langle\sigma_{Y+\xi}\rangle]\to 0 \qquad [42]$$

更多的细节,读者可以参考 Ruelle(1969)和 Gallavotti(1969)的文章。

热力学极限和不等式

格子气模型一个非常有趣的性质就是,在一定程度上它可以用来研究像无限大体积状态是否存在这样的问题。不等式是一种有效的研究工具。作为一个最简单的例子,我们考虑在外场 $h_x\geqslant 0$ 中,相互作用 $J_{xy}\leqslant 0$ 的铁磁伊辛模型:J,b 也许不是变换不变的。那么在"空边界的条件下"(没有外部自旋),$\sigma_X=\sigma_{x1}\sigma_{x2}\cdots\sigma_{xn}$,$X=(x_1,\cdots,x_n)$ 满足不等式

$$\langle\sigma_X\rangle,\partial_{h_x}\langle\sigma_x\rangle,\partial_{J_{xy}}{}^{①}\langle\sigma_X\rangle\geqslant 0,X=(x_1,\cdots,x_n)$$

更一般的,我们将式[39]中的 $H(\sigma)$ 换为 $H(\sigma)=-\Sigma_x J_X\sigma_X$ 其中 $J_X\geqslant 0$ 且 X 为任意有限序列;记 $Y=(y_1,\cdots,y_n)$,$X=(x_1,\cdots,x_n)$,有 Griffiths 不等式:

① J_{xy} 应为 ∂ 的下标,原文似有误——译者注。

$$\langle\sigma_x\rangle \geqslant 0, \partial_{J_Y}\langle\sigma_X\rangle \equiv \langle\sigma_X\sigma_Y\rangle - \langle\sigma_X\rangle\langle\sigma_Y\rangle \geqslant 0 \qquad [43]$$

在铁磁伊辛模型中,我们记边界条件 B 为所有外部自旋都向上或者所有的外部格点全空,那么这个不等式可以用来检验是否存在无限大体积状态(参考"相变与边界条件"和"格点模型"有关章节)。记 $\langle F\rangle_{B,\Omega}$ 为边界条件为 B,任意 $\beta, h>0$ 的条件下巨正则分布的平均值,那么所有的局部观察量 $F(\sigma_\Lambda)$(所有的 F 都依赖於固是区域 Λ 中的自旋构形)的极限都存在

$$\lim_{\Omega \to \infty}\langle F\rangle_{B,\Omega} = \langle F\rangle_B \qquad [44]$$

原因就是不等式[43]表明所有的平均值 $\langle\sigma_X\rangle_{B,\Omega}$ 在 Ω 内对于所有的 $X \subset \Omega$ 都是单调的。所以,极限[44]对于 $F(\sigma)=\sigma_X$ 是存在的。所以,对于所有的仅仅是依赖于有限多的自旋的 F,极限是存在的,因为所有在 Λ 内被测量的 F 都可以表示函数 σ_X 的线性叠加,这里 $X \subseteq \Lambda$ 。

空边界条件下的单调性可按下述方式考察。将 Ω 的尺寸向外扩充一个单位长度的大小,形成一个新的 Ω' ,并想像 J_X 在 $X \in \Omega'$ 而 $X \notin \Omega$ 的区域内为零。那么,$\langle\sigma_X\rangle_{\Omega'} \geqslant \langle\sigma_X\rangle_\Omega$,因为 $\langle\sigma_X\rangle_{\Omega'}$ 是在 $X \in \Omega'$ 而 $X \notin \Omega$ 的区域内根据相互耦合强度为 J_X 的能量进行的平均,能量变化范围是 0 到 $J_X \geqslant 0$。

类似的,如果边界上全是+,那么将 Ω 扩大到 Ω' 则对应着将作用在外部自旋的外场 h 由 ∞(将使所有的自旋全为+)变到一个有限的 $h \geqslant 0$。所以,增加 Ω 将导致 $\langle\sigma_X\rangle_{+,\Omega}$ 减小。所以如果边界条件是空的,那么随着 Ω 的增加,伊辛铁磁自旋的关联也将增加。如果边界是+,关联则减少。

还有很多重要的不等式可以通过简单的途径来证明已经存在的理论。然而不幸的是,它们大都被限制在格点模型,而且它们的能量要做一些特殊的假设(例如上面相互作用的例子)。上面引用的这些例子是首次被发现的,他们为研究非平凡的热力学极限和纯态提供了方法。

更多的细节,读者可以参考 Ruelle(1969),Lebowitz(1974),Gallavotti(1999),Lieb,Thirring(2001),Lieb(2002)的文章。

对称破缺相变

最简单的相变(请看"相变与边界条件"一节)是格点模型中由对称破缺导致的相变。当一个被限制在容器 Ω 内,并且采用特别的边界条件(周期、准周期、空边界条件)的系统的能量对于一个作用在相空间的群 G 具有不变性,则这种相变将会发生。也就是说,γ 是群 G 内的一个元素,它作用在相空间中的一个点 x 上,将 x 映射为 $x\gamma$,这种变换满足群的法则 $(x\gamma)\gamma' \equiv x(\gamma\gamma')$ 。如果 F 是一个可观测量,那么群对相空间的作用将导致 F 由 $F(x)$ 变到 $F_\gamma(x)=F(x\gamma^{-1})$。

在选取合适的边界条件和热力学极限下,一些可观测量对于某些群元素表现出了不对称性,$\langle F\rangle \neq \langle F_\gamma\rangle$。

以简单的 d 维近邻铁磁伊辛模型为例,式[39]给出了能量表达式,这里 $h=0$ 且 $\varphi(x-y)\equiv 0$ 除非 $|x-y|=1$,即 x, y 是近邻格点时,$\varphi(x-y)=J>0$。在周期或者空边界条件下,系统有自旋向上,向下的对称性 $\boldsymbol{\sigma} \to -\boldsymbol{\sigma}$。

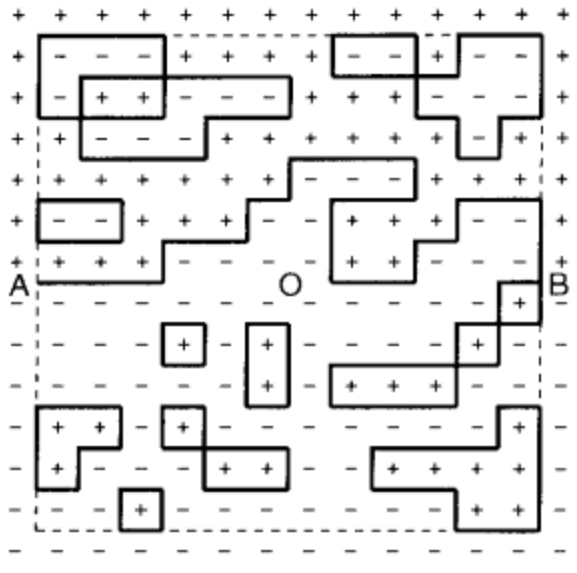

图 2　虚线是 Ω 的边界，外部的自旋对应着±边界条件，A，B 两点是直线 λ 的端点。

通过考虑这样一个边界条件，在 Ω 外的格点或者被＋，或者被－占据，我们可以看到由边界条件带来的不稳定性。我们在考虑这样的两种边界条件，(1)在边界的上半部分是自旋向上，下半部分自旋向下，我们把这种边界条件定义为±边界条件(见图 2)。(2)Ω 的一些相对的边是全同的，其他边被＋或者－占据，我们称它为“圆柱型”或者准周期边界条件。

采用一种新的对自旋构形的描述方式是很有意义的。给定构形 $\boldsymbol{\sigma}$，对两端自旋相反的每一条边 b，在其中心画一条与其垂直的单位长度的线段。我们以±边界条件为例在图 2 中画出了示意图。

这些线段的集合可根据它们来自于正自旋区域或负自旋区域而分组成分离不同区域的线。如果边界条件是＋或者－，那么这些线将组成闭合的多边形。然而，如果边界条件是±，将存在一个多边形 λ_1 是不闭合的。如果边界条件是周期的或者圆柱型的，则所有的多边形都闭合，但是有些会贯穿整个 Ω。这些多边形也叫做“轮廓线”，多边形 γ 的长度被记为 $|\gamma|$。

关于对应 $(\gamma_1,\gamma_2,\cdots,\gamma_n,\lambda_1)\leftrightarrow\boldsymbol{\sigma}$，对于边界条件是＋(或者－)，$\boldsymbol{\sigma}\leftrightarrow(\gamma_1,\cdots,\gamma_n)$ 是一一对应的。如果 $h=0$，这个构形的能量 $H_\Omega(\boldsymbol{\sigma})$ 将比 $-J\times$(Ω 内所有边数的和)多一个量 $2J(|\lambda_1|+\Sigma_i|\gamma_i|)$，或者，$2J\Sigma_i|\gamma_i|$。在 $h=0$ 时每个自旋构形的巨正则分布几率正比于

$$\mathrm{e}^{-2\beta J(|\lambda_1|+\Sigma_i|\gamma_i|)}\quad 或\quad \mathrm{e}^{-2\beta J\Sigma_i|\gamma_i|} \tag{45}$$

式[45]也反映出了系统的自旋上-下的对称性。

在＋的边界条件下，σ_+ 的平均值 $\langle\sigma_x\rangle_{\Omega,+}$ 是 $\langle\sigma_x\rangle_{\Omega,+}=1-2P_{\Omega,+}(-)$，这里 $P_{\Omega,+}(-)$ 是 σ_x 为－1 的几率。如果格点 x 被一个向下的自旋占据，那么这个格点就在所考虑的自旋构形 σ 相应的某个轮廓线的内部。所以，如果给定轮廓线(γ)属于描述构形 $\boldsymbol{\sigma}$ 的轮廓的集合的几率为 $\rho(\gamma)$，那么我们有 $P_{\Omega,+}(-)\leqslant\Sigma_{\gamma ox}\rho(\gamma)$，这里 γox 表明 γ 包围 x。

如果 $\Gamma=(\gamma_1,\cdots,\gamma_n)$ 是一个自旋构形，符号 $\Gamma_{\mathrm{comp}}\gamma$ 表示轮廓 γ 不属于 $\gamma_1,\cdots,\gamma_n$，也就是说 $\gamma\cup\Gamma$ 是一个新的自旋构形，那么

$$\rho(\gamma)=\frac{\Sigma_{\Gamma\ni\gamma}\mathrm{e}^{-2\beta J\Sigma_{\gamma'\in\Gamma}|\gamma'|}}{\Sigma_\Gamma\mathrm{e}^{-2\beta J\Sigma_{\gamma'\in\Gamma}|\gamma'|}}\equiv\mathrm{e}^{-2\beta J|\gamma|}\,\frac{\Sigma_{\Gamma\mathrm{comp}\gamma}\mathrm{e}^{-2\beta J\Sigma_{\gamma'\in\Gamma}|\gamma'|}}{\sum_\Gamma\mathrm{e}^{-2\beta J\Sigma_{\gamma'\in\Gamma}|\gamma'|}}\leqslant\mathrm{e}^{-2\beta J|\gamma|} \tag{46}$$

式[46]最后一个比值没有超过 1。注意到，有 $>3^p$ 个半径为 p 的不同形状的 γ；且其中只有至多 p^2 个包含 x 的全等的 γ。所以当边界条件为＋，发现在格点 x 的自旋为-的几率满足

$$P_{\Omega,+}(-)\leqslant\sum_{p=4}^{\infty}p^2 3^p\mathrm{e}^{-2\beta J p}\xrightarrow[\beta\to\infty]{}0$$

这个几率可以足够小，所以只要 β 足够大，$\langle\sigma_x\rangle_{\Omega,+}$ 可以被估计为 1，而且这个值与 x，Ω 无关。

对于边界条件为-或者 $h=0$ 的相似讨论知，则有 $\langle\sigma_x\rangle_{\Omega,-}=-\langle\sigma_x\rangle_{\Omega,+}$。由此得出，只要有足够大的 β，$\langle\sigma_x\rangle_{\Omega,-}\neq\langle\sigma_x\rangle_{\Omega,+}$ 而且这两个量之间的差在 Ω 中一致地正。这就是，当 β 足够大，磁化强度对边界条件的强烈不稳定性的存在可被证明(Peierl 理论)，也就是最近

邻相互作用二维(或更高维数,相同的理由)伊辛模型具有相变。如果维数是 1,则不发生相变(参考"$d=1$:无相变"一节)。

更多的细节见 Gallavotti(1999)。

有限体积效应

上一节对近邻伊辛模型的描述可以更准确一些,从而可从数学和物理两个方面给出关于相变性质的启示。假设边界条件是(+)的边界,并且描述一个自旋的位形 $\boldsymbol{\sigma}$ 的是相应的一些不相交的闭合多边形($\gamma_1,\cdots,\gamma_n$)。归于 $\sigma=(\gamma_1,\cdots,\gamma_n)$ 的几率正比于[45]。那么,下面的明罗斯-西奈(Minlos-Sinai)定理成立:

定理 如果 β 足够大,存在 $C>0$ 和 $\rho(\gamma)>0$,且有 $\rho(\gamma)\leqslant \mathrm{e}^{-2\beta|\gamma|}$,使得由巨正则系综中随机选取、具有+边界条件和 $h=0$ 的自旋构型 σ,将以 $\Omega\to\infty$ 时接近 1 的几率包含 $K_{(\gamma)}(\sigma)$ 个与 γ 全等的轮廓线,使

$$|K_{(\gamma)}(\boldsymbol{\sigma})-\rho(\gamma)|\boldsymbol{\Omega}||\leqslant \boldsymbol{C}\sqrt{|\boldsymbol{\Omega}|}\,\mathrm{e}^{-\beta|\gamma|} \qquad [47]$$

且这个关系同时对所有的 γ 都成立。

因此,有非常少的大轮廓线(轮廓线越大,数量就越少,不论是绝对或相对值):巨正则系综中一个具有+边界条件的典型自旋构形的大多数自旋是"正",在正自旋的"海"里,有少量的负自旋分布在小而少的区域里(然而,它们的数量仍然具有 $|\Omega|$ 的量级)。

在上一节,另一个分析的结果涉及接近相变区域低温和有限 Ω 时的近似状态方程。如果 Ω 有限,h 对 $m_\Omega(\beta,h)$ 的图将会有相当不同的行为,依赖于可能的边界条件。例如,如果边界条件是(+)或(−),我们分别得到结果如图 3(a)和 3(b)所示,这里 $m^*(\beta)$ 是指自发磁化强度(也就是 $m^*(\beta)\overset{\text{def}}{=}\lim_{h\to 0^+}\lim_{\Omega\to\infty} m_\Omega(\beta,h)$)。

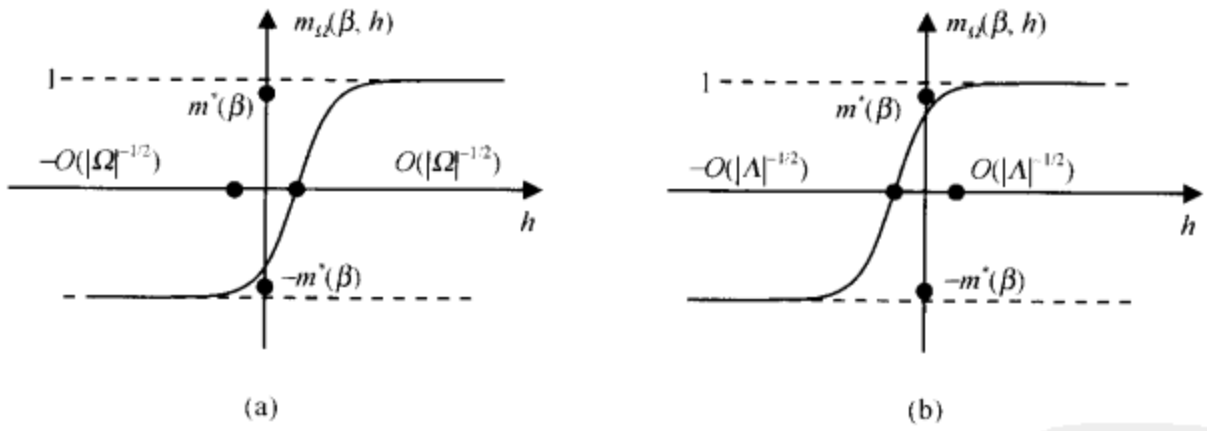

图 3 h 关于 $m_\Omega(\beta,h)$ 的图对于 Ω 有限和(a)+和(b)−的条件。

在周期或自由边界条件,相图就像图 4 中那样变化。热力学极限 $m(\beta,h)=\lim_{\Omega\to\infty} m_\Omega(\beta,h)$ 对所有 $h\neq 0$ 存在,并且在图 4(b)显示了,在 $h=0$ 极限不连续。能够证明,如果 β 足够大,以至于有 $\infty>\lim_{h\to 0^+}\partial_h m(\beta,h)=\chi(\beta)>0$(即图的垂直部分与剩下部分夹角是尖锐的)。

进一步还可以证明,对于不为零的 h,$m(\beta,h)$ 是 h 的解析函数。如果 β 足够小,解析性对所有 h 都成立。对于大的 β,函数 $f(\beta,h)$ 在 $h=0$ 有一个本质的奇异点,这结果可被解释为排除了亚稳态朴素理论,它就是由 $f(\beta,h)$ 到 h 负值的解析延续得到的一个状态方程来决定。

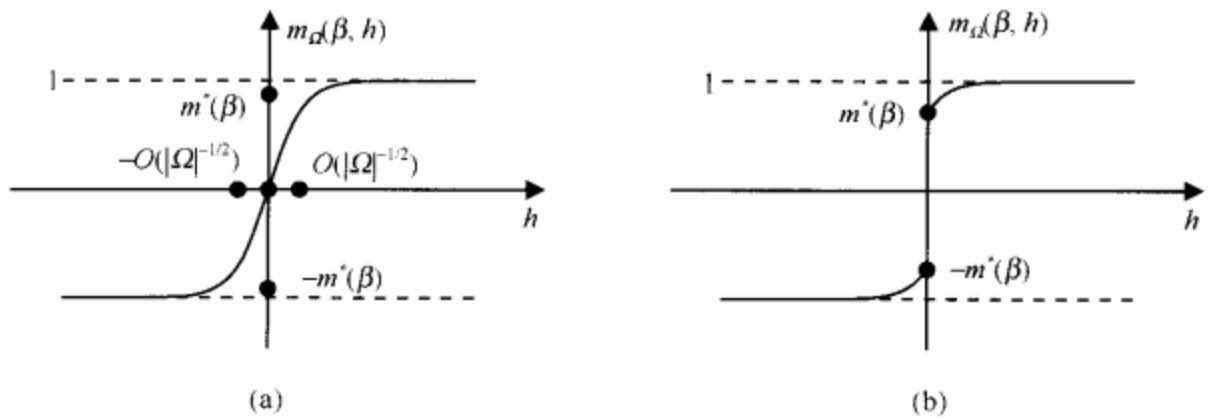

图 4 (a)h 关于 $m_\Omega(\beta,h)$ 的图对于周期或自由边界条件,(b)热力学极限的不连续($h=0$)。

以上的考虑和结果进一步澄清有限系统的相变意义。更多细节,读者可参考 Gallavotti(1999)和 Friedli,Pfister(2004)。

超出低温(铁磁伊辛模型)

上面讨论的结果局限于低温条件(β 足够大)。一个自然的问题就是走出低温区域,在边界条件不稳定性发生和首先发展的区域,完全的描述这个现象。已经知道一些有趣的部分结果,这些明显改善了前面分析得出的物理图像。紧跟着这些结果的一个显著、但远没有详尽的目录,集中在铁磁伊辛自旋系统的性质。局限于这个情形的原因,是它们简单得足以进行一个非常仔细的分析,这个分析清楚地显示统计力学的结构,并可以用来理解更一般的系统。

(1) 让 $z\overset{\text{def}}{=}e^{\beta h}$,并考虑 z^V(V 是 $|\Omega|$ 位置的数目)和周期边界或理想壁边界条件配分函数的乘积,以及铁磁相互作用的范围有限,但不必是近邻相互作用。我们得到一个 z 的多项式($2V$ 阶)。它的零点处在单位圆 $|z|=1$ 上:这就是李-扬定理,它意味着 $f(\beta,h)$ 在区域 $0<\beta<\infty$,$-\infty<h<+\infty$ 的奇异性仅能在 $h=0$ 找到。

如果点 $z=1$ 是一个在单位圆上零点极限分布($\Omega\to\infty$)的聚点,奇异性就能够出现。如果零点是 $z_1,\cdots,z_{2V}$,那么

$$\frac{1}{V}\lg z^V Z(\beta,h,\Omega,\text{周期}) = 2\beta J+\beta h+\frac{1}{V}\sum_{i=1}^{2V}\lg(z-z_i)$$

并且如果

$$V^{-1}\times(z_j=e^{\theta_j}(\theta\leqslant\theta_j\leqslant\theta+d\theta)\text{ 的零点数})\xrightarrow[\Omega\to\infty]{}\frac{d\rho_\beta(\theta)}{2\pi}$$

就有

$$\beta f(\beta,h) = 2\beta J+\frac{1}{2\pi}\int_{-\pi}^{\pi}\lg(z-e^{\theta})d_{\rho_\beta}(\theta) \qquad [48]$$

由热力学极限的存在可得到测度 $d_{\rho_\beta}(\theta)$ 的存在,但是 $d_{\rho_\beta}(\theta)$ 不必是 $d\theta$ 连续,也就是不必正比于 $d\theta$。

(2)可以证明,不必是近邻相互作用,配分函数零点对势能小扰动没有移动太多,即使能量(在理想壁或周期边界条件)被微扰成为

$$H'_\Omega(\boldsymbol{\sigma}) = H_\Omega(\boldsymbol{\sigma})+(\delta H_\Omega)(\boldsymbol{\sigma})$$

$$(\delta H_\Omega)(\sigma)=\sum_{X\subset\Omega}J'(X)\sigma_X \qquad [49]$$

其中 $J'(X)$ 非常一般,被定义在子集 $X=(x_1,\cdots,x_k)\subset\Omega$,使得量 $\|J'\|=\sup_{y\in Z^d}\sum_{y\in X}|J'(X)|$ 足够小。更精确地说,以一个固定的铁磁势 J,假设我们知道当 $J'=0$,配分函数变量 $z=e^{\beta h}$ 的零点处在 z 平面某一个(单位圆的)紧致集 N。然后,如果 $J'\neq 0$,它们处在紧致集 N^1,这个紧致集是 Ω 独立的,并被包含在 N 的附近。当 $\|J'\|\to 0$,其宽度收缩到 0。这允许建立解析性质和下面(3)描述的边界条件不稳定性之间的各种关系。

(3)在铁磁伊辛模型,不必是一个近邻相互作用,如果在 $\theta=0$ 附近 $d_{\rho_\beta}(\theta)=0$,在零附近有一个间隙。可以被证明,如果 β 足够小,对于所有 h 存在着一个宽度一致的间隙。

(4)另一个问题是,是否边界的不稳定性总是可以由单自旋关联函数(即通过磁化强度)来揭示,或者只能通过更高阶的关联函数来体现。可以证明对于 $h\neq 0$ 没有边界不稳定发生,而在 $h=0$ 是可能的,但只有

$$\lim_{h\to 0}m(\beta,h)\neq\lim_{h\to 0+}m(\beta,h) \qquad [50]$$

(5) Griffiths 不等式(参看"热力学极限和不等式"一节)的一个结果是,如果对于给定 β_0,式[50]是对的,那么它对于所有 $\beta>\beta_0$ 都成立。因此,(4)给出了临界点 T_c 的一个自然定义,至少是 T 的上限,使得式[50]有效($k_BT=\beta^{-1}$)。

(6) 如果 $d=2$,近邻铁磁伊辛模型的自由能在 β_c 有奇异点,并且从模型的精确解 $m(\beta,0^+)\overset{\text{def}}{=}m^*(\beta)\equiv(1-\sinh^4 2\beta J)^{1/8}$ 可以精确知道 β_c 的值。对于 $d=3$,作为 β 的函数,$f(\beta,0)$ 奇异性的位置和性质仍是一个未解决的问题。特别是,$f(\beta,0)$ 在 $\beta=\beta_c$ 是否有一个奇异点也是未解决的问题。

(7) 对于 $\beta<\beta_c$,存在对边界条件的不稳定性(见上面(6)),同时有一个自然的问题:铁磁伊辛模型有多少个"纯"相能够存在(参看"相变与边界条件"一节方程[22])? 直觉暗示,应该只存在两相:正磁化相和负磁化相。

人们必须区分平移不变的纯相和平移可变的相。能够证明的是,对于二维近邻铁磁伊辛模型,所有无限大体积的态(参看"格点模型"一节)是平移不变的。进一步,它们可以从考虑只有两个边界条件+和−得到,对于非近邻铁磁相互作用的模型,后者的态也是纯态。这个问题的解已经导致在统计力学和概率论许多新的想法和技巧的引入。

(8) 对于任意 $d\geqslant 2$ 的维数,在 β 足够大时,能够证明近邻伊辛模型只有两个平移不变的相。如果维数 $d\geqslant 3$ 和 β 非常大,+和−的相使平移不变相消失,出现了平移可变的相。然而,从 β 接近 β_c 的问题是十分困难的。

更多的细节,参考 Onsager(1944), Lee, Yang(1952), Ruelle(1971), Sinai(1991), Gallavotti(1999), Aizenman(1980), Higuchi(1981)和 Friedli, Pfister(2004)。

相共存的几何

经典相变现象的直观通常是基于气液相变的性质。实验上研究这个相变通常是在粒子数固定(正则系综)和有外场(重力)的条件下。

这些实验条件有十分重要的影响:外场产生了非平移不变的环境和两相分离。实际

上,固定的粒子数决定了两相各自所占的体积比例。

再次考虑近邻铁磁伊辛模型:对于一些问题我们能获得一个明确的图像,而这些问题对于其他许多模型,以现今技术还是不能了解的。

在固定磁化强度(参看"晶格模型"一节式[40])的正则系综分布下,讨论相共存是比较简单的。让 β 足够大到在两相区域,并且给定一个 $\alpha\subset(0,1)$,让

$$m = \alpha m^*(\beta) + (1-\alpha)(-m^*(\beta) = (1-2\alpha)m^*(\beta) \qquad [51]$$

即 m 有 $m=m(\beta,h)$ 在固定的 β 在图的垂直部分(参看图 4)。

固定 m 在式[51]不产生相被分离在两个不同的区域;对于这个效果,有必要引入一些外在因素导致一个相倾向在某一部分空间中出现。这样的不对称至少有两种方法可得到它:通过不均匀的外场(完全类似于气液相变中的重力场)或通过不对称的场作用于边界的自旋。后者在定性上和前者有相同的效果,因为边界微扰在相变区域产生了体积效应(参看"相变和不等价性"和"对称性破缺与相变"一节)。从数学的观点来看,用边界不对称来产生相分离是比较简单的。最简单的几何形状是考虑±圆柱或++圆柱的边界条件:这说明++或±的边界条件的周期在一个方向上(参看图 2,在去除边界上的自旋以后想象左和右的边界被等同起来)。

把邻接于 Ω 基的自旋作为对称破缺的外场。++的圆柱边界条件倾向于产生在 Ω 内部正的磁化相;因此,在正则分布下仅当总磁化强度固定为自发磁化强度 $m^*(\beta)$ 时,我们才会自然地考虑这一边界条件。

另一方面,±的边界条件倾向相分离(正磁化相在 Ω 的顶部,而负磁化相在其底部)。因此,对正则分布有磁化强度 $m=(1-2\alpha)m^*(\beta)$,$(0<\alpha<1$(式[51])),我们自然会考虑此种边界条件。此时,在一定意义上正相被期待靠近 Ω 的顶部并扩展到 $O(L)$ 距离之处,然后改变成负磁化的纯相。

为了使唯象的描述更加精确,通过相应的不相交的多边形之集合(参看"对称破缺与相变"一节)来考虑自旋构形 $\boldsymbol{\sigma}$。固定边界条件为++或±圆柱边界条件,并注意到与自旋构形 $\boldsymbol{\sigma}$ 相应的多边形是闭的,并分成两种类型:第一类,记为 $\gamma_1,\cdots,\gamma_n$,是不环绕 Ω 的多边形;第二类,记为 λ_a,是至少环绕 Ω 一次的多边形。

所以一个自旋构形 $\boldsymbol{\sigma}$ 将被描述成为一系列多边形;一个构形 $\sigma=(\gamma_1,\cdots,\gamma_n,\lambda_1,\cdots,\lambda_h)$ 的统计权重是(参看式[45]):

$$e^{-2\beta J(\Sigma_i|\gamma_i|+\Sigma_j|\lambda_j|)} \qquad [52]$$

环绕圆柱 Ω 的轮廓线用 λ(而不是 γ)的原因是,若我们忘记 Ω 的对边被等同起来,那么它们看起来就像是开轮廓线(参看"对称破缺与相变"一节)。在±的边界条件下 λ 类型的多边形的数量必须是奇数(因此 $\neq 0$),对于++的边界条件多边形的数量必须是偶数(因此可能是 $=0$)。

更多的细节,参考 Sinai(1991)和 Gallavotti(1999)。

相分离和共存

在上一节自旋构形的几何描述里,我们考虑了正则分布有++圆柱或±圆柱的边界条件和零外场:这里各自简写为 $\mu_{\beta,++}$,$\mu_{\beta,\pm}$。下面的定理(明罗斯-西奈定理)提供了共存相微观理论的基础(建立在维数 $d=2$ 上,但是经过明显改造后对于 $d\geqslant 2$ 也成立)。

定理 对于固定的 $0<\alpha<1$,令 $m=(1-2\alpha)m^*(\beta)$;那么对于 β 足够大一个自旋构形 $\boldsymbol{\sigma}=(\gamma_1,\cdots,\gamma_n,\lambda_1,\cdots,\lambda_{2h+1})$ 按照分布 $\mu_{\beta,\pm}$ 随机选择时下述性质(i)—(iv),在 $\Omega\to\infty$ 时其成立的 $\mu_{B,\pm}$ 几率接近 1:

(i)$\boldsymbol{\sigma}$ 只包括一个 λ 类型的轮廓线,并且有

$$\big||\lambda|(1+\epsilon(\beta))L\big|<o(L) \qquad [53]$$

这里 $\epsilon(\beta)>0$ 是一个 β 的适当函数(与 α 无关),当 $\beta\to\infty$ 时指数趋近零。

(ii) 如果 $\Omega_\lambda^+,\Omega_\lambda^-$ 各自定义为在 λ 之上和之下的区域,并且 $|\Omega|\equiv V$,$|\Omega^+|$,$|\Omega^-|$ 表示 Ω,Ω^+,Ω^- 的体积,这时

$$\begin{aligned}\big||\Omega_\lambda^+|-\alpha V\big|&<\kappa(\beta)V^{3/4}\\ \big||\Omega_\lambda^-|-(1-\alpha)V\big|&<\kappa(\beta)V^{3/4}\end{aligned} \qquad [54]$$

这里 $\kappa(\beta)\xrightarrow[\beta\to\infty]{}$ 指数衰减;这里和下面的指数 3/4 都不是最优的。

(iii) 如果 $M_\lambda^+=\sum_{x\subset\Omega_\lambda^+}\sigma_x$ 和 $M_\lambda^-=\sum_{x\subset\Omega_\lambda^-}\sigma_x$,则

$$\begin{aligned}|M_\lambda^+-\alpha V|&<\kappa(\beta)V^{3/4}\\ |M_\lambda^--(1-\alpha)V|&<\kappa(\beta)V^{3/4}\end{aligned} \qquad [55]$$

(iv) 如果 $K_\lambda^\gamma(\boldsymbol{\sigma})$ 是指全等于给定 γ 且处于 Ω_λ^+ 中轮廓线的数目,那么对所有该种形状的 γ 都有

$$|K_\gamma^\lambda(\boldsymbol{\sigma})-\rho(\gamma)\alpha V|\leqslant Ce^{-\beta l|\gamma|}V^{1/2},C>0 \qquad [56]$$

这里 $\rho(\gamma)\leqslant e^{-2\beta l|\gamma|}$ 与"有限体积效应"定理已提到的量是一样的。对 λ 之下的轮廓线有一个相似的结果(参看关于式[47]的注解)。

上面的定理不仅提供了一个细节和更满意的对于相分离现象描述,而且也提供了两相分离线的精确微观定义,应当把它与(随机)λ 线等同。

正则分布 $\mu_{\beta,++,m^*(\beta)}$ 有相似的结果,这里(i)被非 λ 类型多边形所代替,同时(ii),(iii)成为多余的,(iv)要被明显修改。换句话说,分布 $\mu_{\beta,++,m^*(\beta)}$ 典型的构形与带+的边界条件的巨正则系综的典型位形(它的性质由"超出低温(铁磁伊辛模型)"一节的定理描述)有相同的结构。

更多的细节,见 Sinai(1991)和 Gallavotti(1999)。

相分离线和表面张力

继续考察近邻伊辛铁磁体模型,上一节的定理说明,如果 β 足够大,这时分离两相的微观线 λ 几乎是直的(因为 $\epsilon(\beta)$ 很小)。微观线 λ 与直线的偏离在带±边界条件的巨正则分布 $\mu_\pm^0$ 下最便于研究,而该边界条件是指在 $\partial\Omega$ 包括垂直部分的上半平面上设成+1,且在其下半平面部分设成−1。关于该边界条件的说明见图 2(参看"对称破缺与相变"一节)。相关的结果可转成上一节带±圆柱型边界条件的巨正则分布的相似结果。

定义 λ 是**刚性的**如果 λ 通过盒子 Ω(即 0)中心的几率当 $\Omega\to\infty$ 时不趋于 0;否则就**不是刚性的**。

刚性的概念区分了线 λ 是"直线"的可能性。"额外"的长度 $\epsilon(\beta)L$(见式[53])可以从两个方法得到:或者线 λ 基本上是直的(在几何意义下),但带有一些密度为 $\epsilon(\beta)$ 的分布其上的"凹凸"或者它仅仅局部是直的,但由于小的弯折而在大尺度上累积出十分重要的额

外长度。在三维相似的现象是可能的。λ 的刚性或没有刚性在原则上可以由光学手段来研究;只要 λ 在上述意义下是刚性的,通过宏观上 λ 分离的表面元散射的相干光就有干涉现象。

已经严格证明了二维的 λ 线不是刚性的。并且至少在低温中间点的涨落是 $O(L)$ 的量级。然而在三维已经证明,当温度充分低时曲面 λ 是刚性的。

更进一步的分析需要研究在其他条件下(例如。带+边界条件的正则分布且磁化强度介于 $\pm m^*(\beta)$ 之间)分离表面的形状。作为先来条件这涉及两相之间表面张力的定义和许多性质。此处,我们仅提及带+边界条件的二维情况下表面张力的定义。如果 $Z^{++}(\Omega, m^*(\beta))$ 和 $Z^{+-}(\Omega, m)$ 各自是++和±圆柱边界条件下的正则配分函数,则张力 $\tau(\beta)$ 定义为

$$\beta\tau(\beta) = -\lim_{\Omega\to\infty}\frac{1}{L}\lg\frac{Z^{+-}(\Omega, m)}{Z^{++}(\Omega, m^*(\beta))}$$

对于足够大的 β,极限是独立于 α 的:定义及其合理性基于"相共存几何"一节中的微观几何描述。定义能够自然的扩展到更高的维数去(和更一般的非近邻的模型)。如果 $d=2$,张力 τ 在低于临界温度的全部温度下都能够被精确计算出来,是 $\beta\tau(\beta) = 2\beta J + \lg\tanh\beta J$。

更重要的是,定义可以扩展到在"方向 n"定义表面张力 $\tau(\beta, n)$,这里边界条件使得分离线平均上垂直单位矢量 $\boldsymbol{n}$。这样,如果 $d=2$ 和 $\alpha\subset(0,1)$ 是固定的,能够证明,在足够低的温度和+边界条件及介于磁化强度 $m=(1-2\alpha)m^*(\beta)$ 时正则分布有典型的构形包括一个面积约 αV 的负自旋区域;进一步,如果容器被重新标度为 $L=1$,这个区域将会有一个充满区域 α 的限定形状,而区域 α 可用以表面张力 $\tau(n)$ 为术语来描述晶体形状的经典宏观乌尔夫(Wulff)理论决定的光滑曲线所包围。

在三维情况,还有一个没有解决的有趣问题:可以想像尽管在低温分离表面是刚性的,但在温度 $\tilde{T}_c$ 略微低于临界温度 T_c(后者被定义为低于它就会出现两个纯相的最高温度)可能变"软"。其存在性已很好地建立在数值实验基础上的温度 $\tilde{T}_c$ 被称为"粗略相变"温度。λ 的刚性与非平移不变平衡态的存在相联系。后者在 $d=3$ 存在,但是在 $d=2$ 不存在已讨论过的 λ 非刚性,建立了到 $\tilde{T}_c$ 的所有途径,并给出了不出现非平移不变态的直观原因。在 $d=3$,粗略温度 $\tilde{T}_c(\beta)$ 不能小于有相同耦合的二维伊辛模型的临界温度。

注意到,平移不变平衡态的存在性不必描述共存现象。近邻二维伊辛模型理论清楚地证明了这个说法。

更多的细节,读者可以参考 Onsager(1944), van Beyeren(1975), Sinai(1991), Miracle-Sole(1995), Pfister, Velenik(1999),以及 Gallavotti(1999)。

临界点

对具有短程相互作用且处于平衡态的系统(它是纯相),其关联函数具有团簇特性(见式[22]):其物理意义是,纯相中相距很远的区域的涨落之间互不相关。最简单的团簇性质涉及"对关联函数",即不考虑其他粒子的位置时在点 q_1, q_2 各找到一个粒子的几率密度 $\rho(q_1, q_2)$(见式[23])。对自旋系统,对关联函数则为 $\rho(q_1, q_2) = \langle\sigma_{q_1}\sigma_{q_2}\rangle$。在平移不变

的平衡态中,如果

$$|\rho(q_1,q_2)-\rho^2| \xrightarrow[|q_1-q_2|\to\infty]{} 0 \qquad [57]$$

则对关联具有团簇性质(式[22]和[42]),其中 ρ 是在 q 处找到一个粒子的几率密度(即系统的物理密度),或者 q 处自旋的平均值 $\rho=\langle\sigma_q\rangle$(即磁化强度)。

平衡态可用参数表示,例如巨正则分布的 β,λ,正则分布的 β,ν 以及格点自旋系统巨正则分布的 β,h。临界点的一般定义是参数空间中的一点 c。在只有短程作用(即 $|r|$ 足够大时 $\varphi(r)$ 为零)的系统中,如果对关联函数比指数函数更慢(如距离 $|r|=|q_1-q_2|$ 的幂次函数)的趋于 0(见式[57]),则对应的点 c 是临界点。

一个典型的例子是二维正方格点上近邻相互作用的伊辛模型,它有且仅有一个临界点 $\beta=\beta_c,h=0$,其中 $\sinh 2\beta_c J=1$,J 是相互作用强度。其团簇性质表现为:在 $\beta<\beta_c,\beta>\beta_c$ 和 $\beta=\beta_c$ 时,关联 $\langle\sigma_x\sigma_y\rangle-\langle\sigma_x\rangle\langle\sigma_y\rangle \xrightarrow[|x-y|\to\infty]{} 0$ 依次按

$$A_+(\beta)\frac{e^{-\kappa(\beta)|x-y|}}{\sqrt{|x-y|}},A_-(\beta)\frac{e^{-\kappa(\beta)|x-y|}}{|x-y|^2},A_c\frac{1}{|x-y|^{1/4}} \qquad [58]$$

方式,其中 $A_\pm(\beta),A_c,\kappa(\beta)>0$。性质[58]来自该模型的精确解。

在临界点会发生诸多有趣现象。指数衰减的缺乏表明,不存在一个长度标度,当超过它时会发生截然不同的现象,以及不同尺度上观测的系统性质可能通过适当的标度变换简单的联系起来。人们在如何定量理解不同观测量的标度性质方面做出了诸多努力。结果是发展了临界现象的重整化群的方法(见"重整化群"一节)。出现的图像是:越接近临界点,在这个尺度以下能观测到标度性质的最大尺度越大。例如无外场的格点自旋系统,如果 a 选取适当,在正方体 $\Lambda\subset\Omega$ 中的磁化强度 $M|\Lambda|^{-a}$ 对所有边长小于 $l_0(\beta)$ 的 Λ 有相同的分布,当 $\beta\to\beta_c$ 时 $l_0(\beta)\to\infty$。a 被称为临界指数。

在临界点附近还可定义其他"临界指数",它们与热力学函数的奇异性或者两点或多点关联函数的行为相关。例如格点自旋系统,至少在距离很大但是小于 $l_0(\beta)$ 时,其 $2n(n=1,2,3,\cdots)$ 点自旋关联 $\langle\sigma_0\sigma_{\xi_1},\cdots,\sigma_{\xi_{2n-1}}\rangle_c$ 应该正比于坐标 $(\xi_1,\cdots,\xi_{2n-1})$ 的某种 ω_{2n} 次齐次函数 $\chi_{2n}(0,\xi_1,\cdots,\xi_{2n-1})$,其中

$$l_0(\beta)=\text{常数}\times(\beta-\beta_c)^{-\nu}\xrightarrow[\beta\to\beta_c]{}\infty$$

这表明,如果将 ξ_i 认为是 $\mathbb{R}^d$ 中的点,当 $1\ll|\xi_i-\xi_j|\ll l_0(\beta)$ 时,函数 χ_{2n} 满足

$$\chi_{2n}\left(0,\frac{\xi_1}{\lambda},\cdots,\frac{\xi_{2n-1}}{\lambda}\right)=\lambda^{\omega_{2n}}\chi_{2n}(0,\xi_1,\cdots,\xi_{2n-1}),(0<\lambda\in\mathbb{R}) \qquad [59]$$

同时 $\langle\sigma_0\sigma_{\xi_1},\cdots,\sigma_{\xi_{2n-1}}\rangle\propto\chi_{2n}(0,\xi_1,\cdots,\xi_{2n-1})$。参数 ω_{2n} 定义了一系列的临界指数。

其他临界指数与沿其他方向趋于临界点相联系。如 $\beta=\beta_c$ 而 $h\to0$ 时,具有标度现象的最大尺度为 $l_0(h)=l_0h^{\bar{\nu}}$;此外,磁化强度按 $m(h)=m_0h^{1/\delta}$ 形式趋于 0,其中 $\delta>0$。

包括存在性在内,临界指数的所有特征都不是严格已知。一个例外是二维近邻作用的伊辛铁磁体,其部分指数严格已知(如 $\omega_2=1/4,\omega_{2n}=n\omega_2,\nu=1$ 等),但也有部分指数未严格知道(如 $\delta,\bar{\nu}$ 等)。不过,对于所有维数伊辛铁磁体(不一定是近邻作用,但作用程有限),推测上面提到的所有临界指数与近邻作用的伊辛铁磁体完全相同。另一个例外是临界指数之间严格关系的推导,有些情形下,在假设存在后推导它们的值。

评注 在无外场且 $\langle\sigma_x\rangle=0$ 的纯态中,如果 Λ 是边长为 l 的立方盒子,可以简单地期

望参量 $s=|\Lambda|^{-1/2}\sum_{x\in\Lambda}\sigma_x$ 应具有高斯概率分布,且有色散$\lim_{\Lambda\to\infty}\langle s^2\rangle$。该结论"通常是对的",但并不是总对。性质[58]说明 $d=2$ 近邻相互作用铁磁伊辛模型$\langle s^2\rangle$正比于 $l^{2-\frac{1}{4}}$ 发散,使得参数 s 不可能具有上述的高斯分布。变量 $S=|\Lambda|^{-7/8}\sum_{x\in\Lambda}\sigma_x$ 的色散有限,但是没理由要求它是高斯分布。这表明临界点附近的涨落理论及相关研究非常有趣(见下面两节)。

更多的细节,读者参见文献 Onsager(1994), Domb, Green(1972), McCoy, Wu(1973),及 Aizenman(1982)。

涨落

上节讨论中提到,可观测量在其平均值附近的涨落具有有趣的性质,在临界点尤其如此。特别有趣的是可观测量都是相空间上局部函数 $F(x)$在大体积 Λ 上的平均,这是因为宏观量经常都具有这种形式。例如系统容器 Ω 内给定的区域 Λ,$\Lambda\subset\Omega$,考虑一个构形 $x=(P,Q)$和 Λ 中的粒子数 $N_\Lambda=\sum_{q\in\Lambda}1$,或者势能 $\Phi_\Lambda=\sum_{q,q'\in\Lambda}\varphi(q-q')$ 或者动能 $K_\Lambda=\sum_{q\in\Lambda}(1/2m)p^2$。格点自旋系统情形则考虑一个构形 σ 和 Λ 中的诸如 $M_\Lambda=\sum_{i\in\Lambda}\sigma_i$ 等。将以上 4 个例子依次编号为 $\alpha=1,\cdots,4$。

用 μ_α 表示平衡态的几率分布,考虑变量 X_Λ,记 $x_\Lambda=\langle X_\Lambda/|\Lambda|\rangle_{\mu_\alpha}$,$p\overset{\text{def}}{=}(X_\Lambda-x_\Lambda)/|\Lambda|$。则应该研究的涨落的典型性质是($\alpha=1,\cdots,4$):

(1) 对任意 $\delta>0$,$\lim_{\Lambda\to\infty}\mu_\alpha(|p|>\delta)=0$(大数定理);

(2) 存在 $D_\alpha>0$,使得 μ_α[①]$(p\sqrt{|\Lambda|}\in[a,b])\xrightarrow[\Lambda\to\infty]{}\int_a^b\frac{\mathrm{d}z}{\sqrt{2\pi D_\alpha}}\mathrm{e}^{-z^2/2D_\alpha}$(中心极限定理);

(3) 存在区间 $I_\alpha=(p^*_{\alpha,-},p^*_{\alpha,+})$和凹函数 $F_\alpha(p)$,$p\in I_\alpha$[②],使得$[a,b]\subset I$ 时$\frac{1}{|\Lambda|}\lg\mu_\alpha$[③]$(p\in[a,b])\xrightarrow[\Lambda\to\infty]{}\max_{p\in[a,b]}F_\alpha(p)$(大偏差定理)。

大数定理保证了宏观量的确定性;中心极限定理控制 X_Λ 的小涨落($\sqrt{|\Lambda|}$ 阶)围绕其平均值;而大偏差定理考虑的是$|\Lambda|$ 阶的涨落。

以上关系(1)~(3)并不总是对的。进一步假设粒子系统的势 φ 满足式[14],或者格点自旋系统满足 $\sum_q|\varphi(q)|<\infty$,这些关系可以被证明。函数 $F_\alpha(p)$定义为平衡态 μ_α 对应的适当热力学函数的热力学极限。本质上对所有情形,进一步的假设是对应热力学函数的 $F_\alpha(p)$是光滑的,且有非零的二阶导数。

为了讨论一个简单的具体例子,考虑伊辛模型的格点自旋系统,在巨正则平衡态 $\mu_{h,\beta}$ 中,其能量为 $-\sum_{x,y\in\Omega}\varphi(x-y)\sigma_x\sigma_y-\sum_x h\sigma_x$,磁化强度的涨落为 $M_\Lambda=\sum_{x\in\Lambda}\sigma_x$,$\Lambda\subset\Omega$。

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① 应为 μ_α,原文误为 μ—— 译者注。

② 应为 I_α,原文误为 I——译者注。

③ 应为 μ_α,原文误为 μ——译者注。

记自由能为 $\beta f(\beta,h)$(见式[41]),$m=m(h)\overset{\text{def}}{=}\langle M_\Lambda/|\Lambda|\rangle$,$h(m)$是 $m(h)$的反函数。若 $p=M_\Lambda/|\Lambda|$,函数 $F(p)$为

$$F(p)=\beta(f(\beta,h(p))-f(\beta,h)-\partial_h f(\beta,h)(h(p)-h)) \qquad [60]$$

则一个相当普遍的结论是

定理 当势满足 $\sum_x|\varphi(x)|<\infty$,且 $F(p)$式在[60]所考虑的 p 周围的开区间(确切而言,对大数定理和中心极限定理是 $p=0$ 周围,而大偏差定理是包含 a,b 的开区间)中是光滑函数且 $F''(p)\neq 0$ 时,关系(1)~(3)成立。

在所面临的情形中,系综等价理论意味着函数 F 也能从其他平衡系综自然相关的热力学函数求得。例如不采用巨正则的 $f(\beta,h)$,而考虑正则的 $\beta g(\beta,m)$(见式[41]),则

$$F(p)=-\beta(g(\beta,p-g(\beta,m)-\partial_m g(\beta,m)(p-m)) \qquad [61]$$

必须指出,中心极限定理和大偏差定理之间应该存在很强的关系。撇开严格的数学定理的条件,该论断可有效的用 $\Lambda=\Omega$ 铁磁格点自旋系统来阐明。在外场 h_0 的平均值 $m(h_0)$附近,h_0 附近所有 h 值中心极限定理的有效意味着小间隔大偏差定理的成立,反之亦然。为简单起见,取 $h_0=0$,具有启发意义的原因见下面。记 $\mu_{h,\Omega}$是外场 h 下的巨正则分布,则

(1) 定义几率 $\mu_{h,\Omega}(p\in \mathrm{d}p)$正比于 $\mu_{0,\Omega}(p\in \mathrm{d}p)\mathrm{e}^{-\beta h p|\Omega|}$。因此,如果中心极限定理对 $h_0=0$ 附近所有 h 值都成立,则存在两个在 $h_0=0$ 附近的 h 的函数 $m(h)$和 $D(h)>0$,满足 $m=0$ 和

$$\mu_{0,\Omega}{}^{①}(p\in \mathrm{d}p)e^{-\beta h p|\Omega|}=\text{常数}\times\exp\left(|\Omega|\frac{(p-m(h))^2}{2D(h)}+o(\Omega)\right)\mathrm{d}p \qquad [62]$$

(2) 存在一个函数 $\zeta(m)$使得$\partial_m\zeta(m(h))=\beta h$,$\partial_m^2\zeta(m(h))=D(h)^{-1}$。注意到对给定的 $D(h)$,偏微分方程$\partial_m\beta h=D(h)^{-1}$与初始条件 $h_0=0$ 可以决定函数 $h(m)$;所以 $\zeta(m)$可通过$\partial m\zeta(m)=\beta h(m)$的二次积分得到。

启发性可得到,零外场时 p 的几率具有形式常数$\times^{\zeta(p)|\Omega|}\mathrm{d}p$,从而 $p\in[a,b]$中的几率为常数$\times\exp(|\Omega|\max_{p\in[a,b]}\zeta(p))$。

反之,$h=0$ 时 p 的大偏差定理意味着足够小外场 h 下 p 的涨落满足中心极限定理:这可简单的从函数 $F(p)$的二阶导数为负得到。

这表明中心极限定理和大偏差定理具有对偶性,或者说大偏差定理是中心极限定理的总体版本,从这种意义上说:

(1) 如果中心极限定理对 h_0 附近的 h 成立,则在外场 h_0 下的磁化强度在 $m(h_0)$附近的足够小区间 J 中的涨落满足大偏差定理;及

(2) 如果在 h_0 附近的一个区间内大偏差定理成立,则对 $h-h_0$ 足够小的所有外场 h,磁化强度在其平均值附近的涨落满足中心极限定理。

超越建立对偶性的启发水平,需要进一步给出"足够小"的精确意义,讨论需要用到 $m(h)$,$D(h)$或 $F(p)$的何种性质来推导性质(1)和(2)。

为阐明这点,考虑具有短程作用 φ 的铁磁伊辛模型:则如果 β 足够小,中心极限定理对所有 h 都成立,而大偏差定理对所有 h 和区间$[a,b]\subset(-1,1)$都成立。若果 β 不够小,

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① 应为 $\mu_{0,\Omega}$,原文误为 μ_0—— 译者注。

则需要加上条件 $h\neq 0$。因此该条件相当的弱,同时显然可以期望 $h=0$ 和 β 不够小时,论断不成立,因为此时有可能会发生相变。

发生相变时,大数定理、中心极限定理和大偏差定理需要重新阐述。基本上,必须考虑纯相中的涨落,以一种自然的方式改变定理的阐述。例如,在零外场、大 β 伊辛模型的纯相(即由+或−边界条件、有限体积态取极限得到的状态)中,磁化强度在不包含平均磁化强度 m^* 的区间 $[a,b]$ 中的大涨落不是必必须随尺寸 $|\Lambda|$ 指数减小。如果 $[a,b]\subset[-m^*,m^*]$ 它们随 Λ 的表面(即 $|\Lambda|^{(d-1)/d}$)指数减小,而 $[a,b]\cap[-m^*,m^*]=\phi$ 时它们随体积指数减小。

上节的讨论说明,在临界点大涨落的性质预期也会改变。因为例子[58]中,随着盒子边长趋于∞,磁化强度的正规二阶矩平均值发散,不能期望中心极限定理普遍成立。

更多细节,读者参见文献 Olla(1987)。

重整化群

刚讨论的涨落理论只涉及单个参量的涨落。而多个参量联合涨落的问题也很有意思,事实上,在 20 世纪 70 年代它引发了新的发展。为了阐述方法背后的一些思想和哲理,有必要将注意力集中在一些相当特殊的事例中。因此,考虑一个经典平衡系综对应的平衡分布 μ_0。为了明确想法,我们考虑伊辛能量函数 βH_0 的平衡态分布:能量中包含温度因子是因为我们将讨论 μ_0 作为 β 的函数的性质。同时假定自旋的平均值为零("无磁场",见 $h=0$ 时的式[39])。为了记住一个具体情形,设想 βH_0 就是零场中近邻作用伊辛铁磁体的能量函数。

假设体积为 Ω 的容器具有周期性边界条件,其体积非常大,理想情况下可当作无限大。定义一团块 $k\xi$,它由晶格格点 $x=\{k\xi_i\leqslant x_i<(k+1)\xi_i\}$ 构成,其中参数 $\xi\in\mathbb{Z}^d$,k 为整数。这是一个尺度为 k 的立方块组成的晶格,称为 k 重新标度晶格。

对给定 α,物理量 $m_\xi=k^{-\alpha d}\sum_{x\in k\xi}\sigma_x$ 被称为团块自旋。定义映射 $R^*_{\alpha,k}\mu_0=$将原始自旋的初始分布转换为块自旋的分布。值得注意的是,如果初始自旋只有两种取值 $\sigma_x=\pm 1$,团块自旋则从 $-k^d/k^{\alpha d}$ 到 $k^d/k^{\alpha d}$ 每间隔 $2/k^{\alpha d}$ 取一个值。另外,映射 $R^*_{\alpha,\kappa}$ 与初始自旋可以取多少个值没有关系,甚至可以假定自旋可取连续值 $S_x\in\mathbb{R}$。

对于大 k,取 $\alpha=1$ 意味着考察团块 $k\xi$ 中的联合大涨落的几率分布,而取 $\alpha=1/2$ 则对应于研究团块变量的联合中心极限特性。

考虑一个以 β(将被视作温度的倒数)作参数的、初始分布为 μ_0 的单参数族。一般而言,有且仅有一个 α 值 $\alpha(\beta)$,使得团块变量的联合涨落满足极限分布

$$\mathrm{prob}_k(m_\xi\in[a_\xi,b_\xi],\sigma\in\Lambda)\xrightarrow[k\to\infty]{}\int_{\{a_\xi\}}^{\{b_\xi\}}q_\Lambda((S_\xi)_{\xi\in\Lambda})\prod_{\xi,M}\mathrm{d}S_\xi,\qquad[63]$$

其中 $q_\Lambda(z)$ 是 $\mathbb{R}^\Lambda$ 上的某个分布。

若 $\alpha>\alpha(\beta)$,该极限为 $\prod_{\xi\in\Lambda}\delta(S_\xi)\mathrm{d}S_\xi$,或者若 $\alpha<\alpha(\beta)$ 时极限不存在(因为块变量将太大,色散随 $k\to\infty$ 发散)。

将 $k\to\infty$ 的序列选取为 $k=2^n$,$(n=0,1,\cdots)$ 比较方便,因为此时 $R^*_{\alpha,\kappa}=R^{*n}_{\alpha,1}$,且沿序列 $k=2^n$ 的极限 $k\to\infty$ 可认为是映射 $R^*_{\alpha,1}$ 的迭代序列的极限,而认为 $R^*_{\alpha,1}$ 作用于格点 $\mathbb{Z}^d$

中的通有的自旋 S_x 的几率分布(序列 3^n 同等适用)。

更加方便的是将几率分布用能量函数 H 表示,其中 H 在热力学极限下可产生一个分布 μ。则 $R^*_{\alpha,1}$ 可定义一个作用于能量函数的操作 R_α,使得 $R_\alpha H=H'$ 其中 H 产生 μ、H' 产生 μ'、$R^*_{\alpha,1}\mu=\mu'$。当然能量函数比式[39]更普遍,且至少必须承认一个形如式[49]中 δU 的形式。

换言之,作用于能量函数的操作 R_α 给出了操作 $R^*_{\alpha,1}$ 的结果。其迭代定义了一个半群,称为团块自旋重整化群。

尽管几率分布的映射 $R^*_{\alpha,1}$ 确实定义明确,但并不意味着能量函数的映射 R_α 也定义明确。因为如果 μ 由一个能量函数给定,但并不清楚 $R^*_{\alpha,1}\mu$ 是否也如此。

当 $R^*_{\alpha,1}$ 及其迭代作用在短程作用的自旋系统的高温(小 β)平衡初态 μ_0 上时,可(容易地)证明一个重要的定理。该情形下,若 $\alpha=1/2$,分布 $R^*_{\alpha,1}\mu_0(\beta)$ 的序列满足的极限可用独立的高斯分布的乘积表示:

$$\mathrm{prob}_k(m_\xi\in[a_\xi,\beta_\xi],\sigma\in\Lambda)\xrightarrow[k\to\infty]{}\int_{a_\xi}^{b_\xi}\prod_{\xi\in\Lambda}\exp\left(-\frac{1}{2D(\beta)}S_\xi^2\right)\prod_{\xi\in\Lambda}\frac{\mathrm{d}S_\xi}{\sqrt{2\pi D(\beta)}}\qquad[64]$$

注意到陈述该定理时甚至都没提到重整化映射 $R^n_{1/2}$,不过这可以解释成

$$R^n_{1/2}\beta H_0\xrightarrow[n\to\infty]{}\sum_{\xi\in\mathbb{Z}^d}\frac{1}{2D(\beta)}S_\xi^2\qquad[65]$$

但是该解释并不严格,因为[64]没有表明要求 $R^n_{1/2}\beta H_0$ 当 $n\geqslant 1$ 时有意义。它表明团块自旋在高温时有正态的独立涨落,因此是中心极限定理的推广。

存在几种情形,至少当 R_α 作用在诸如自旋系统高温态的特殊平衡态时,可严格证明映射 R_α 定义明确。但这都是些相对无趣的特殊情形。

不过,有大量的文献处理映射 R_α 的近似表示。原因在于,假设作用于有限区域的映射存在且具有预期的性质后,由此可得到许多结果。其中一个非平凡结果是得到了第一个超出范德瓦耳斯理论(见"范德瓦耳斯"一节)的临界点理论。

本质上可如下进行讨论。从 $<\left(\sum_{x\in\Lambda}\sigma_\xi/\sqrt{|\Lambda|}\right)^2>$ 趋于∞ 的意义上说,临界点的涨落预期是反常的(见"临界点"一节最后一个评注)。因为 $\alpha=1/2$ 不对应 $\sum_{\xi\in\Lambda}\sigma_\xi$ 的正确涨落标度,表明 $R^{*n}_{1/2,1}\mu_0(\beta_c)$ 不具有极限。但是存在 $\alpha_c>1/2$,使得 $R^*_{\alpha_c,1}\mu_0(\beta_c)$ 在式[63]的意义上收敛到一个极限。近邻相互作用伊辛铁磁情形下 $\alpha_c=7/8$(见"临界点"一节最后的注释)。因此,如果认为映射 $R^*_{\alpha_c,1}$ 作用于 $\mu_0(\beta)$,则对所有 $\beta<\beta_c$,$R^{*n}_{\alpha_c,1}\mu_0(\beta$[①]$)$会收敛到一个平凡的极限 $\prod_{\xi\in\Lambda}\delta(S\xi)\mathrm{d}S\xi$,因为对正常的涨落 α_c 值大于 1/2。

如果认为映射 R_{α_c} 能作用于能量函数,这表明 $\prod_{\xi\in\Lambda}\delta(S_\xi)\mathrm{d}S_\xi$ 是"重整化群"的一个"平凡不动点",它"吸引"能量函数 βH。到高温相对应的能量函数。

临界 β_c 的存在与 R_{α_c} 的"非平凡不动点 H^*"的存在密切相关,该不动点是双曲的仅有一个李雅普诺夫指数 $\lambda>1$,因此它有一个余维数为 1 的稳定流形。称 μ^* 为 H^* 对应的几率分布。

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① 应为 β,原文误为 β_c。——译者注。

$\beta<\beta_c$ 时向平凡不动点的移动可简单解释如下：该 β 值下的初始能量函数 βH_0 处于非平凡不动点的稳定流行之外，在重整化群 R_{α_c} 作用下，βH_0 向吸引所有方向的平凡不动点移动。

当 β 升高至 $\beta=\beta_c$ 时，βH_0 可能会穿过 R_{α_c} 的非平凡不动点 H^* 的稳定流形。则 $R^n_{\alpha_c}\beta_c H_0$ 不再趋于平凡不动点，而是趋于 R_{α_c} 的非平凡不动点 H^*。这表明团块自旋变量出现完全不同的涨落行为。当 β 接近 β_c 时，R_{α_c} 的迭代会使得 $R^n_{\alpha_c}\beta_c H_0$ 接近 H^*，直到最终又沿不稳定方向排开，可达到的最近距离随 $\lambda^n|\beta-\beta_c|$ 增大。

这意味着在某特征尺度之下的涨落会趋于稳定不动点的分布 μ^*，而之上则趋于平凡不动点，该特征尺度为 $O(2^{n(\beta)})$ 个格点单位，其中 $\lambda^{n(\beta)}|\beta-\beta_c|=1$，因此也即 $O(|\beta-\beta_c|^{-\lg_2\lambda})$。为看到这点，团块自旋必须用指标 $\alpha=1/2$ 归一化，它们表现为独立的高斯涨落（见式[64]和[65]）。

接下来的问题是如何找到非平凡的不动点，也就是找到 R_{α_c} 的不动点的能量函数 H^* 及对应 α_c。如果以上图像是正确的，H^* 对应的分布 μ^* 可描述临界涨落。如果 α_c 和 H^* 只有一个或有限个选择，则会打开一扇通往临界点普适理论的大门，正如范德瓦耳斯理论的“原始”结果所暗示的那样。

最初的希望可能是只存在很少的可能临界值 α_c 和 H^*，但临界涨落可分为不同普适类的可能性很快减小。每类都包含众多的能量函数，在 R_{α_c} 的迭代作用下，当 β 小时被（总存在的）平凡不动点控制，而 $\beta=\beta_c$ 时被具有相同的 α_c 和 H^* 的 R_{α_c} 的非平凡不动点 H^* 控制。对 $\beta<\beta_c$，趋于平凡不动点的重新处理可通过考虑 $R_{1/2}$ 而不是 R_{α_c} 看到，它的迭代会导致如式[64]的高斯分布（以及如式[65]的极限能量函数）。

该图像有很强的假设性，但它是第一个提出可得到临界点普适特性的物理机制，其临界指数不同于范德瓦耳斯理论及其格点铁磁版本（居里-外斯理论）。此外，从定义明确的 $R^*_{\alpha,1}$ 转到作用于能量函数的 R_α 需要做近似（如威尔逊-费希尔 ϵ 展开），承认这些近似就有可能得到明确的 α_c 的值和 H^* 的表达式，具体与作用在不同类模型上的 R_{α_c} 有关。

例如，由此可推断短程铁磁作用的所有自旋系统（其能量函数由式[39]给出）具有由相同的 α_c 和非平凡不动点决定的临界点。这个性质虽远未从数学上证明，但被认为是该理论的最大成功。与范德瓦耳斯临界点理论比较，这是历史上第一次给出了可计算且与范德瓦耳斯理论不同的临界指数，尽管其近似甚至并不完全可控。

临界现象的重整化群方法有多种变体，这取决于考虑何种涨落和应用于何种模型。在统计力学中，有一些数学上的完全应用：某些高维结果、$d=2$ 维偶极子气体理论，等级模型、凝聚态和格点自旋统计力学的一些问题和一些其他问题。其主要数学成功发生在各种相关领域，不仅上面描述的思想可以应用，而且得到了精确定义并可具体研究的重整化变换，例如结构场论、准周期运动的 KAM 理论和动力学系统中的不同问题。

然而应用总涉及具体情形，且每种情形中似乎都会出现平凡-非平凡不动点两分性的一般图像。但是除极少情形（如层次模型，或者区间映射普适理论）外，并不伴随着关于稳定流形、不稳定方向和不直接感兴趣的重整化变换作用的完整描述（一般性看起来经常是一个棘手的问题，但并不必都如此）。

以重整化群为背景，在提供普适类并不很少的清楚证据方面，数学物理扮演了重要角

色。这从近邻相互作用伊辛铁磁的 Onsager 解之后大量严格解可以看出。事实上,存在几种二维格点模型,其临界点具有可精确计算的临界指数,并连续依赖于模型参数。

更多细节,读者参见文献 McCoy, Wu(1973), Baxter(1982), Bleher, Sinai(1975), Wilson, Fisher(1972), Gawedzky, Kupiainen(1983, 1985), Benfatto, Gallavotti(1995),以及 Mastropietro(2004)。

量子统计

统计力学可以相当直接地被推广到量子粒子的集合。在 N 个全同粒子的情形下,可观测量是希尔伯特空间上的算子 O,它们张成的希尔伯特空间是

$$\mathcal{H}_N = L_2(\Omega)_a^N \quad 或 \quad \mathcal{H}_N = (L_2(\Omega) \bigotimes C^2)_a^N$$

其中 $a=+,-$ 分别对应着对称($a=+$,玻色系统)和反对称($a=-$,费米系统)的波函数。对于只考虑粒子位置 $Q=(q_1,\cdots,q_N)$ 的波函数 $\psi(Q)$ 与同时考虑粒子位置 Q 和自旋 $\sigma=(\sigma_1,\cdots,\sigma_N)$ 的波函数 $\psi(Q,\sigma)$,分别有它们的归一化条件:

$$\int |\psi(Q)|^2 \mathrm{d}Q = 1 \quad 或 \quad \sum_\sigma \int |\psi(Q,\sigma)|^2 \mathrm{d}Q = 1$$

这里只考虑 $\sigma_j=\pm 1$。同在经典统计中一样,我们用可观测量的系综平均值 $\langle O\rangle$ 来定义宏观状态。

我们可以很容易地对量子系统定义微正则、正则、巨正则系综。比如,对于一个哈密尔顿如下的系统:

$$H_N = -\frac{\hbar^2}{2m}\sum_{j=1}^N \Delta_{q_j} + \sum_{i<j}\phi(q_j - q_j') + \sum_j w(q_j) \stackrel{\mathrm{def}}{=} K + \Phi \qquad [66]$$

这里我们要求系统 Ω 满足周期性边界条件,同时外势 $w(q)$ 是光滑的周期函数,对于非零的 w 而言,我们还要求系统的周期长度是外势周期的倍数。我们可以给出这个系统的可观测量 O 在具有逆温度 β 和单位体积 $v=V/N$ 的正则系综中的系综平均值

$$\langle O\rangle \stackrel{\mathrm{def}}{=} \frac{\mathrm{tr}\ \mathrm{e}^{\beta H_N} O}{\mathrm{tr}\ \mathrm{e}^{-\beta H_N}} \qquad [67]$$

对于巨正则系综的平衡态,我们可以类似地给出定义。

值得注意的是,这几个系综是等价的,"热学定理"能够被证明(见"热学定理和遍历假设"一节)。然而,均分性不成立,即 $\langle K\rangle \neq (d/2)N\beta^{-1}$。尽管 β^{-1} 仍然是热学定理中 $\mathrm{d}U+p\mathrm{d}V$ 的积分因子,从而 β^{-1} 仍然正比于温度。

均分性的缺失这点是非常重要的,它解决了经典统计中我们处理无穷多自由度系统时常会碰见均分性问题造成的佯谬,比如(用相互耦合振子组成的晶格来描述)晶体或者场(例如,在研究黑体辐射时很重要的电磁场)。然而,这已经是量子统计给我们的第一个惊喜(事实上导致了量子的发现),但绝不是最后一个。

低温时,会出现新的、没有料想到的(没有经典统计力学对应的)现象。例如,玻色-爱因斯坦凝聚(超流),费米面的不稳定性(超导),以及非对角长程序的出现。它们给出了量子统计中本质上和经典统计不同的问题。这些现象提出了非常有趣的问题,不仅从物理的观点,从数学的观点上看也是如此。很多问题现在仍然没有得到很好的解释,甚至在定义的层面都还没有解决。但是,我们应该记住,在我们感兴趣的情形(即三维系统,甚至大

部分的二维或者一维系统），对于类似式[66]的系统，能证明下面定义的现象真正存在（注意最后的评注，有一个重要的例外）。

玻色-爱因斯坦凝聚

在具有参数 β,v 的正则系综态上，用 $L_2(\Omega)$ 上核 $\rho(q,q')$ 的本征值 $\nu_j(\Omega,N)$ 定义玻色-爱因斯坦凝聚的出现，被称为单粒子约化密度矩阵，并被定义为

$$N\sum_{n=1}^{\infty}\frac{\mathrm{e}^{-\beta E_n(\Omega,N)}}{\mathrm{tr}\,\mathrm{e}^{-\beta H_N}}\int\bar{\psi}_n(q,q_1,\cdots,q_{N-1})\psi_n(q',q_1,\cdots,q_{N-1})\mathrm{d}q_1\cdots\mathrm{d}q_{N-1} \qquad [68]$$

这里 $E_n(\Omega,N)$ 是 H_N 的本征值，$\psi_n(q_1,\cdots,q_N)$ 是相应的本征态。如果让 $\nu_j(\Omega,N)$ 按升序排列，在固定的 $v=V/N,\beta$，若对于所有大 Ω，有 $\nu_1(\Omega,N)\geqslant bN>0$，则我们称在这个具有参数 β,v 的宏观态上发生了玻色-爱因斯坦凝聚。这个定义可解释为系统有超过 bN 个粒子具有相同的动量。在固定密度和低温时，自由玻色气系统存在玻色-爱因斯坦凝聚现象。

费米面

波函数 $\psi_n(q_1,\sigma_1,\cdots,q_N,\sigma_N)\equiv\psi_n(Q,\sigma)$ 在对换两个粒子 (q_i,σ_i) 的变换下反对称。让 $\psi(Q,\sigma;N,n)$ 标记式[66]中 N 粒子能量 H_N 的第 n 个本征值为 $E(N,n)$ 的本征函数（由 $n=0,1,\cdots$ 标示和以升序排列）。令 $Q=(q_1'',\cdots,q_{N-p}''),\sigma''=(\sigma_1'',\cdots,\sigma''_{N-p})$。由

$$\rho_p(Q,\sigma;Q',\sigma')\overset{\mathrm{def}}{=}p!\binom{N}{p}\int\sum_{\sigma''}\mathrm{d}^{N-p}Q''\sum_{n=0}^{\infty}\frac{\mathrm{e}^{-\beta E(N,n)}}{\mathrm{tr}\,\mathrm{e}^{-\beta H_N}}$$
$$\times\bar{\psi}(Q,\sigma;Q'',\sigma'';N,n)\psi(Q,\sigma;Q'',\sigma'';N,n) \qquad [69]$$

引入被称为 p 粒子约化密度矩阵的核 $\rho_p^{H_N}(Q,\sigma;Q',\sigma')$（推广对应的单粒子密度约化矩阵[68]）。记 ρ_1[①]$(q_1-q_2)\overset{\mathrm{def}}{=}\sum_{\sigma}\rho_1(q_1,\sigma,q_2,\sigma)$，考虑无自旋费米系统同样有意义，相应的定义通过去掉自旋指标可得到，下面不再重复说明这一点。

记 $\rho_1(q-q')$ 的傅里叶变换为 $r_1(k)$，于是可以利用它来定义费米面。当 $\Omega\to\infty,\beta\to\infty$ 时，我们称 $\partial_k\gamma_1(k)$ 在其邻域中无界的 k 之轨迹为费米面。$\beta\to\infty$ 下的极限是重要的，因为费米面的概念可能仅在零温时是准确的，即在 $\beta=\infty$。

目前为止，在自由费米系统（$\varphi=0$）中被证明了存在费米面（即除了在 k 空间光滑表面以外，$r_1(k)$ 是光滑的），还有（1）某些精确可解的一维无自旋模型，（2）更广泛一些的一维无自旋模型，以及有两体排斥相互作用的自旋模型，有的含周期外势。

由于和晶体里的传导理论有关，大家最感兴趣的是在周期外势作用下含自旋的二维或更高维模型。本质上来讲，对于我们上面提到的模型，对于维数 $d>1$ 的情况，没有可用的数学结果。这是这个理论还存在的问题，也是对我们的挑战。

在二维或更高的维数，对于哈密尔顿为[66]的费米系统，没有可用的结果存在，无自旋时情况一样。甚至不清楚有相互作用时费米面能够存在。

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① 应为 ρ_1，原文误为 ρ—— 译者注。

库珀对

超导理论唯象地将超导与库珀对的存在联系起来。考虑式[66]中的哈密尔顿,对照式[69]定义

$$\rho(x-y,\sigma;\ x'-y',\sigma;\ x'-x') \overset{\text{def}}{=} \rho_2(x,\sigma,y,-\sigma;\ x',\sigma',y',-\sigma')$$

如果存在函数 $g^{\alpha}(q,\sigma)\neq 0$ 满足

$$\int g^{\alpha}(q,\sigma)g^{\alpha'}(q,\sigma)\mathrm{d}q = 0 \quad \text{如果 } \alpha \neq \alpha'$$

使得

$$\lim_{V\to\infty}\rho(x-y,\sigma,x'-y',\sigma',x-x') \xrightarrow[x-x'\to\infty]{} \sum_{\alpha} g^{\alpha}(x-y,\sigma)\,\bar{g}^{\alpha}(x'-y',\sigma') \quad [70]$$

则称系统包含具有自旋 $\sigma,-\sigma(\sigma=+$ 或 $\sigma=-)$ 的库珀对。在这情况下,在归一化后,具有最大 L_2 模的 $g^{\alpha}(x-y,\sigma)$ 被称为最低配对能量态的波函数。这和自由粒子的平面波形式类似,而且与之一样,这个波函数明显也是不可归一化的,作为 x,y 的函数,它不是平方可积的。如果系统中存在库珀对,而且在式[70]的极限下,非首项足够快地趋向于零,那么二粒子约化密度矩阵[70]作为一个核算子,在 $V\to\infty$ 时,有一个 V 阶的本征值。也就是说,最低能量态被"宏观占据"了,与自由玻色子凝聚在基态颇为类似。

由于库珀对的不稳定性,在一些情况下,费米面不再存在,即 $r_1(\boldsymbol{k})$ 是 $\boldsymbol{k}$ 的解析函数;同样,在存在库珀对的情况下,由 $r_1(\boldsymbol{k})$ 的奇异点的轨迹组成的表面仍然存在。在前一种情况中,费米面奇异性的痕迹仍然存在,即在某些区域,$r_1(\boldsymbol{k})$ 具有非常陡的梯度,在这里梯度指数依赖于耦合强度的倒数。这就是 BCS 超导理论预言的现象。但是,这个模型是一个平均场模型,可能这个奇异性消失是它的特性之一。在任何情况下,对于一些我们关心的密度矩阵,光滑的奇异点表面都很有可能存在(例如,在具有"带参数 γ"的 BCS 模型中,库珀对的最低能级波函数

$$g(x-y,\sigma) \equiv \frac{1}{(2\pi)^d}\int_{\varepsilon(k)>0} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(x-y)}\,\frac{\gamma}{\sqrt{\varepsilon(\boldsymbol{k})^2+\gamma^2}}\mathrm{d}\boldsymbol{k}$$

在与自由系统费米面一致的表面上是奇异的)。

非对角长程序

考虑 k 费米子约化密度矩阵 $\rho_k(Q,\sigma;Q',\sigma')$,它可以被看作空间 $L_2((\Omega\times C^2)^k)$ 的核算子 O_k。当 k 为偶数时,我们称系统具有 k 阶**非对角长程序**,只要当 $N\to\infty, N/V=\rho$ 时,O_k 具有广义的阶数为 $N^{k/2}$ 的本征值。对于奇数的 k,非对角长程序的定义变成,具有 $N^{(k-1)/2}$ 阶的本征值。当然,这里的 $k\geqslant 3$($k=1$ 时,O_1 最大的本征值必然不大于 1)。

对于玻色子,我们将约化密度矩阵 $\rho_k(Q;Q')$ 视作 $L_2(\Omega)^k_+$ 上的核算子 O_k。于是我们称系统存在 k 阶非对角长程序,只要当 $N\to\infty, N/V=\rho$ 时,$O(k)$ 具有广义的 N^k 阶本征值。

非对角长程序可看作是玻色-爱因斯坦凝聚和库珀对的统一,玻色-爱因斯坦凝聚对应于式[68]中的核子符 $\rho_1(q_1-q_2)$,这个算符具有 N 阶广义本征值,是一阶非对角长程序的情形。如果这是一个具有集团性质意义的纯态(见"相变和边界条件"与"格点模型"一节),那么非对角长程序、玻色-爱因斯坦凝聚以及库珀对的存在都意味着系统发生了自发对称性破缺。粒子数守恒和聚团意味着,由具有哈密顿量[66]和周期性边界条件的状

态极限实现的态相距无限远,所有约化密度矩阵的非对角元为零。这与非对角长程序不一致。

自由费米气没有非对角长程序,超导 BCS 模型具有库珀对和 $k=2$ 的非对角长程序,但是不再存在以上意义的费米面(也许太绝对)。费米系统不可能有一阶非对角长程序(因为单粒子约化密度矩阵的界限是 1)。

在提供精确可解模型方面,数学物理做出特别有效的贡献,但是这些可解模型处理的是一维系统,可以证明,在一维、二维系统中,没有非对角长程序存在。最近的主要进展就是,对一个特殊密度和 $d\geqslant 3$ 的格点形式[66],证明了非对角长程序和玻色凝聚。

对于哈密尔顿为式[66]的系统,在 $\varphi\neq 0$ 的情况下,对于 $d>1$ 还没有任何关于库珀对存在或者费米面存在的证明。不过,在一些极限情况,玻色-爱因斯坦凝聚或者库珀对的形成能够被严格证明。一旦上面提到的这些发生,我们相信,有不少现象也会随之发生,如哈密尔顿量的简单谱性质。有一些已经在具体的模型中得到了验证。

当 $d=1,2$ 时,利用波哥留波夫不等式(在"连续对称性:无 $d=2$ 晶体原理"一节中被用到过),可以证明,在 $T>0$ 不可能存在非对角长程序。

更多的细节,读者可参见文献 Onsager(1956),Yang(1962),Ruelle(1969),Hohenberg(1967),Gallavotti(1999)及 Aizenman et al. (2004)。

附录一:稳定性条件的物理意义

如果稳定性和缓增性条件(见式[14])被破坏,考察会发生什么是有用的。这个分析还可展示统计力学的一些典型方法。

短程吸引造成的结合灾难

当相互作用势 φ 在原点处光滑且为负值时,式[14]第一个条件被最简单破坏。

让 $\delta>0$ 是如此之小,使得在距离 $\leqslant 2\delta$ 的相互作用势 $\leqslant -b<0$。考虑体积为 V 正方形盒子 Ω 中具有参数 β,N 的正则系综分布,所有 N 个粒子处在盒子中心(或盒子中任意一个预先确定的点)附近半径为 δ 小球内的几率为 P_{collapse};注意到

$$\Phi\leqslant -b\binom{N}{2}\sim -\frac{b}{2}N^2$$

可以估算出

$$\begin{aligned} P_{\text{collapse}} &= \frac{\int_c \frac{\mathrm{d}p\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta(K(p)+\Phi(q))}}{\int \frac{\mathrm{d}p\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta(K(p)+\Phi(q))}} \\ &\geqslant \frac{\left(\frac{4\pi\sqrt{2m\beta^{-1}}}{3h^3}\right)^N \frac{\delta^{3N}}{N!}e^{\beta b(1/2)N(N-1)}}{\int \frac{\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta\Phi(q)}} \end{aligned} \qquad [71]$$

这相空间特别小。然而,这样构形比宏观看起来正常的构形出现的可能性大许多。宏观看起来正常的构形即粒子以平均间距 $(N/V)^{-1/3}=\rho^{-1/3}$ 宏观地均匀分布在整个空间的构形,对某个 u,它们的能量 $\Phi(q)$ 具有 uN 的量级,以至于它们的几率具有上限

$$P_{\text{regular}} \leqslant \frac{\int \frac{\mathrm{d}p\mathrm{d}p}{h^{3N}N!}\mathrm{e}^{-\beta(K(p)+uN)}}{\int \frac{\mathrm{d}p\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta(K(P)+\Phi(q))}}$$

$$= \frac{\frac{V^N\ \sqrt{2m\beta^{-1}}^3}{h^{3n}N!}\mathrm{e}^{-\beta uN}}{\int \frac{\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta\Phi(q)}} \qquad [72]$$

然而,不管 δ 有多小,当 $V\to\infty$, $N/V\to v^{-1}$ 时,$P_{\text{regular}}/P_{\text{collapse}}$ 很快地趋向于零。这发生的非常快,因为 $\mathrm{e}^{\beta bN^2}/2$ 最终控制了 $V^N\sim\mathrm{e}^{N\lg N}$。

所以,在一个微观尺度 δ 的空间找到系统的几率比宏观能量正比于粒子数 N 的构形的概率大许多。这被称为紫外灾难(这是由于非常短距离的行为),当 $V\to\infty$ 时,它引起粒子塌陷集中在任意小区域的构形。

长程吸引造成的结合灾难

接近∞时相互作用势吸引太强,这就会发生。为简单起见,假设相互作用势中有硬核项,也就是说,在 $r<r_0$ 时,相互作用变成 $+\infty$。在这种情况下,粒子密度存在上限,即 $\rho_{cp}<\infty$(最紧密排列密度),我们上面提到的紫外灾难不再发生。

当 $|q|$ 很大时,若 $\varphi(q)\sim-g|q|^{-3+\varepsilon}$,其中 $g,\varepsilon>0$,这时会发生我们这里讨论的长程灾难。引力相互作用就是一例:记引力常数为 k,粒子质量为 m,这时,$g=km^2$ 及 $\varepsilon=2$。

与其邻近粒子距离是 $\rho^{1/3}$ 阶的"正则构形"的几率 P_{regular},将与平均密度为 $\rho_{cp}/(1+\delta)^3$、粒子与其邻近粒子距离为 γ。并几乎紧密堆积的"塌陷构形"的几率 P_{collapse} 相比较,这里 γ_0 等于硬核半径乘以 $1+\delta$。在塌陷情况下,系统粒子不能填满其有效体积,由此留下一个空的区域,它在 V 占 $\sim((\rho_{cp}-\rho)/\rho_{cp})V$ 的体积。

我们可以进一步验证,当 $\delta>0$ 足够小(且 $\rho<\rho_{cp}$)的时候,$P_{\text{regular}}/P_{\text{collapse}}$ 以 $O\left(\exp\left(g\frac{1}{2}N(\rho_{cp}(1+\delta)^{-3}-\rho)\right)\right)$ 的方式趋向于零。

由此可知,一个系统在无穷远处大吸引,它将不占据全部的有效体积,甚至在空的地方它也将被约束而处于紧密堆积的构形。

这对于星球理论非常重要,我们可不指望星球遵从"正常的热力学",特别星球不会蒸发掉,因为在大距离,它们的粒子通过引力相互作用。星球不会占据给它们的整个体积(也就是宇宙)。仅因为相互作用有一个很强排斥核,它们不会塌陷到一个点(甚至当它们被燃尽,辐射压不足以保持它们一个合理尺寸)。

蒸发灾难

这是另一种**红外灾难**,即一种由于上面小节粒子间相互作用长程结构导致的灾难。它发生在相互作用势在∞太排斥了,即

$$\varphi(q)\sim+g|q|^{-3+\varepsilon}\quad \text{当 } q\to\infty$$

以至于缓慢性条件又被破坏。

在这种情况中,粒子同样不会占据整个空间,它们形成以紧密堆积构形粘在容器壁上

的一个粒子层。所以,如果密度比紧密堆积密度低,即 $\rho<\rho_{cp}$,系统将会在容器 Ω 的中心区域留下空位,空区域的体积仍和盒子的总体积同阶(即它的直径将是盒子边长 L 的一个分数)。除了最低能量的构形是粒子粘在容器壁且紧密堆积而不是紧密堆积在中心外,这种情况下的证明和我们上一节做的证明完全类似。

这个灾难对于现实中同种电荷组成的系统很重要。电荷以紧密堆积构形附着在系统边界上,以此配置它们使得系统的静电势能最小。所以,电荷配置在金属表面,而不是占据整个空间,它们在表面层状分布,以使得势能最小(于是内部的库仑势为常数)。一般来说,非中性电荷并不对热力学造成影响,比如,它们并不占据所有给它们的空间,于是它们不像通常情况下对比热做出贡献。

中性系统的电荷对热力学有贡献,当它们有硬核或者遵从量子力学对费米子的要求的时候,紫外灾难也不会出现(对于带同种电荷的玻色子同样适用)。

更多的细节,读者参见文献 Lieb,Lebowitz(1972),Lieb,Thirring(2001)。

附录二:子系可加性方法

一个假定性的简单结论是,式[10]中的指数的上限是 $e^{\beta BN}\exp\left(-\frac{\beta}{2m}\sum_{i=1}^{N}\boldsymbol{P}_i^2\right)$。于是有

$$1\leqslant Z_{gc}(\beta,\lambda,V)\leqslant \exp(Ve^{\beta\lambda}e^{\beta B}\sqrt{2m\beta^{-1}}^{d})$$

$$\Rightarrow 0\leqslant \frac{1}{V}\lg Z_{gc}(\beta,\lambda,V)\leqslant e^{\beta\lambda}e^{\beta B}\sqrt{2m\beta^{-1}}^{d} \qquad [73]$$

为简单起见,考虑有限作用程的硬核相互作用(比较式[14])。考虑一组边长为 2^nL_0 的盒子 Ω_n,这里 L_0 为任意固定数且$>2R$。对应于体积 Ω_n 的配分函数 $Z_{gc}(\beta,z)$ 是

$$Z_n=\sum_{N=0}^{\infty}\frac{z^N}{N!}\int_{\Omega_n}\mathrm{d}Q e^{-\beta\Phi(Q)}$$

这是因为,对变量 $\boldsymbol{P}$ 的积分可以明确地完成,如果 z 被定义为 $z=e^{\beta\lambda}(2m\beta^{-1})^{d/2}$,则它可以包含在 z^N 里。

对于 $n\geqslant 1$,编号为 Ω_n 的盒子里含有 2^d 个 Ω_{n-1} 的盒子,而且有

$$1\leqslant Z_n\leqslant Z_{n-1}^{2^d}\exp(\beta B 2d(L_{n-1}/R)^{d-1}2^{2d}) \qquad [74]$$

这是因为,在可填满 Ω_n 的 2^d 个立方体 Ω_{n-1} 的边界上宽度为 $2R$ 区域的体积是 $2RL_{n-1}2^d$,最多包含有 $(L_{n-1}/R)^{d-1}2^d$ 个粒子。每个粒子最多与其他 $2d$ 个其他粒子有相互作用。对于某个 $\gamma_d>0$,所以有

$$\beta p_n\overset{\mathrm{def}}{=}L_n^d\lg Z_n\leqslant L_{n-1}^d\lg Z_{n-1}+\beta B\gamma_d 2^{-n}(L_0/R)^{d-1}$$

对于某个 $\Gamma_d>0$ 和被 n 上下一致限制着的 p_n,有 $0\leqslant\beta p_n\leqslant\beta p_{n-1}+\Gamma_d 2^{-n}$。所以,对序列 $L_n=L_0 2^n$ 极限[13]存在,并可以定义函数 $\beta p_\infty(\beta,\lambda)$。

一个任意边长 L 的盒子可以被 $(L/L_{\bar{n}})^d$ 个边长为 $L_{\bar{n}}$ 的盒子填满。取 $\bar{n}$ 足够大,使得对所有 $n\geqslant\bar{n}$ 和预先确定的 $\delta>0$ 有 $|p_\infty-p_n|<\delta$。同样的,如果 n 很大,边长为 L_n 的盒子可以被 $(L_n/L)^d$ 个边长为 L 的盒子填满。后一个评论使我们得出结论,通过标准不等式,式[13]的极限存在,而且与 p_∞ 一致。

刚才对有限作用程硬球相互作用势展示的子系可加性方法,可以被推广到满足稳定性和缓增性的相互作用势(参见"热力学极限"一节)。

更多的细节,读者参见文献 Ruelle(1969)及 Gallavotti(1999)。

附录三:红外不等式

红外不等式来自于博戈留波夫不等式。考虑"连续对称性:无 $d=2$ 晶体定理"一节讨论的结晶问题作为一个例子。对于具有给定温度 β 和密度参数 $\rho=a^{-3}$ 及哈密尔顿量

$$H=\sum_{j=1}^{N}\frac{p_j^2}{2}+U(Q)+\varepsilon W(Q)$$

的系统,用 $<\cdot>$ 表示正则系综平衡态的平均值。设 $\{X,Y\}=\sum_j(\partial_{pj}X\partial_{qj}Y-\partial_{qj}X\partial_{pj}Y)$ 为泊松括号。在周期性边界条件下,进行分部积分得到一般等式

$$\langle A^*\{C,H\}\rangle\equiv-\frac{\int A^*\{C,\mathrm{e}^{-\beta H}\}\mathrm{d}P\mathrm{d}Q}{\beta Z_c(\beta,\rho,N)}$$

$$\equiv-\beta^{-1}\langle\{A^*,C\}\rangle \qquad [75]$$

对于 $A=\{C,H\}$,后一个等式意味着

$$\langle\{H,C\}^*\{H,C\}\rangle=-\beta^{-1}\langle\{C,\{H,C^*\}\}\rangle \qquad [76]$$

所以,施华兹不等式 $\langle A^*A\rangle\langle\{H,C\}^*\{H,C\}\rangle\geqslant|\langle\{A^*,C\}\rangle|^2$ 与式[75],[76]中两关系结合,得出博戈留波夫不等式

$$\langle A^*A\rangle\geqslant\beta^{-1}\frac{|\langle\{A^*,C\}\rangle|^2}{\langle\{C,\{C^*,H\}\}\rangle} \qquad [77]$$

令 g,h 为任意复(可微)函数,且记 $\partial_j=\partial_{q_j}$ 以及

$$A(Q)\overset{\mathrm{def}}{=}\sum_{j=1}^{N}g(q_i),\quad C(P,Q)\overset{\mathrm{def}}{=}\sum_{j=1}^{N}p_jh(q_j) \qquad [78]$$

如果

$$\Phi(q_1,\cdots,q_N)=\frac{1}{2}\sum_{j\neq j'}\varphi(|q_j-q_j'|)+\varepsilon\sum_j W(q_j)$$

那么有 $H=\sum\frac{1}{2}p_j^2+\Phi(q_1,\cdots,q_N)$。令 $h_j\overset{\mathrm{def}}{=}h(q_j)$,通过代数计算有

$$\{C,H\}\equiv\sum_j(h_j\partial_j\Phi-p_j(p_j\cdot\partial_j)h_j)$$

如果 h 是实数,再经过代数计算,$\langle\{C,\{C^*,H\}\}\rangle$ 成为

$$\Big\langle\sum_{jj'}h_jh_{j'}\partial_j\cdot\partial_{j'}\Phi(Q)\Big\rangle+\Big\langle\varepsilon\sum_j h_j^2\Delta W(q_j)+\frac{4}{\beta}\sum_j(\partial_jh_j)^2\Big\rangle$$

(对 p_j 的积分只是用 $2\beta^{-1}$ 替换 p_j^2,$\langle(p_j)_i(p_j)_{i'}\rangle=\beta^{-1}\delta_{i,i'}$)。所以平均值 $\langle\{C,\{C^*,H\}\}\rangle$ 成为

$$\Big\langle\frac{1}{2}\sum_{jj'}(h_j-h_{j'})^2\Delta\varphi(|q_j-q_{j'}|)+\varepsilon\sum_j h_j^2\Delta W(q_j)+4\beta^{-1}\sum_j(\partial_jh_j)^2\Big\rangle \qquad [79]$$

选取 $g(q)\equiv\mathrm{e}^{-i(\kappa+K)\cdot q}$,$h(q)=\cos(q\cdot\kappa)$,取 $(h_j-h_j)^2$ 的界为 $\kappa^2(q_j-q_{j'})^2$,$(\partial_jh_j)^2$ 的界为 κ^2,h_j^2 的界为 1。所以,式[79]以 $ND(\kappa)$ 为上界,这里

$$D(\kappa) \stackrel{\text{def}}{=} \left\langle \kappa^2 \left(4\beta^{-1} + \frac{1}{2N} \sum_{j \neq j'} (q_j - q_{j'})^2 \, | \Delta\varphi(q_j - q_{j'}) | \right) + \varepsilon \frac{1}{N} \sum_j | \Delta W(q_j) | \right\rangle \quad [80]$$

这可以被用来估计式[77]中的分母。式[77]的左边为

$$\langle A^*, A \rangle = \left| \sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}q \cdot (\kappa + K)} \right|^2$$

和

$$\begin{aligned} |\langle \, |A^*, C| \, \rangle|^2 &= \left| \left\langle \sum_j h_j \partial g_j \right\rangle \right|^2 \\ &= |K + \kappa|^2 N^2 (\rho_\varepsilon(K) + \rho_\varepsilon(K + 2\kappa))^2 \end{aligned}$$

在两边乘上一个辅助函数 $\gamma(\kappa)$(假定它为偶函数,且当 $|\kappa| > \pi/a$ 的时候为零),对 κ 求和,于是式[77]变成

$$\begin{aligned} D_1 &\stackrel{\text{def}}{=} \frac{1}{N} \sum_\kappa \gamma(\kappa) \left\langle \frac{1}{N} \left| \sum_{j=1}^{N} \mathrm{e}^{-i(K+\kappa) \cdot q_j} \right|^2 \right\rangle \\ &\geqslant \frac{1}{N} \sum_\kappa \gamma(\kappa) \frac{|K|^2}{4\beta} \frac{(\rho_\varepsilon(K) + \rho_\varepsilon(K + 2\kappa))^2}{D(\kappa)} \end{aligned} \quad [81]$$

为了应用式[77]、式[80]和式[81]的平均值必须有上限,这是需这里讨论的技术要点,它说明了利用热力学极限和它们的凸性的结果获得估计的一般方法。

注意到

$$\left\langle (1/N) \sum_\kappa \gamma(\kappa) \mathrm{d}^d\kappa \left| \sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}\kappa \cdot q_j} \right|^2 \right\rangle$$

与

$$\tilde{\varphi}(0) + (2/N) \left\langle \sum_{j<j'} \tilde{\varphi}(q_j - q_{j'}) \right\rangle$$

相等,其中

$$\tilde{\varphi}(q) \stackrel{\text{def}}{=} (1/N) \sum_\kappa \gamma(\kappa) \mathrm{e}^{\mathrm{i}\kappa \cdot q}$$

令

$$\varphi_{\lambda,\zeta}(q) \stackrel{\text{def}}{=} \varphi(q) + \lambda q^2 \, | \Delta\varphi(q) | + \eta \tilde{\varphi}(q)$$

以及

$$F_V(\lambda, \eta, \zeta) \stackrel{\text{def}}{=} (1/N) \lg Z^c(\lambda, \eta, \zeta)$$

其中 Z^c 是体积为 Ω、能量为 $U' = \sum_{jj'} \varphi_{\lambda,\zeta}(q_j - q_{j'}) + \varepsilon \sum_j W(q_j) + \eta\varepsilon \sum | \Delta W(q_j) |$ 的配分函数。于是 $F_V(\lambda, \eta, \zeta)$ 是 λ, η 的凸函数。如果 $|\eta|, |\varepsilon|, |\zeta| \leqslant 1$,且 $|\lambda| \leqslant \lambda_0$,它还有一致的上下界。如果 $r^2 | \Delta\varphi(r) |$ 满足"连续对称性:'无 $d=2$ 晶体'定理"一节开头所做的假设,而且密度小于紧密堆积密度,那么存在有 $\lambda_0 > 0$(这是因为,在 $|\varepsilon|, |\eta| < 1$ 且 λ 足够小时,势函数 U' 仍一致满足式[14]类似的条件)。

凸性和一个区间内有上下限意味内部点的导数有界,在上述情况,正适合 F_V 对 λ, η, ζ 在 0 处的导数。后者与式[80]和[81]中的平均值相同。用这种方法,找到了满足 $D(\kappa) \leqslant \kappa^2 B_1 + \varepsilon B_2$ 和 $B_0 > D_1$ 的常数 B_1, B_2, B_0。

更多的细节,读者参考文献 Mermin(1968)。

进一步的阅读材料

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导论:泛函分析

导言

泛函分析研究的是函数和函数空间,它的研究综合了来自经典分析和代数的技巧。近代泛函分析的发展是围绕那些其解为函数的解方程问题展开的。在 18 世纪研究了常微分和偏微分方程之后,19 世纪出现了对积分方程和其他泛函方程的讨论,在它的后期就产生了对一种新的分析的需要,这种分析所针对的是具有无穷个变量的函数而不是通常的函数。1887 年,Volterra 受到变分方法的启发,提出一种新的无穷小方法,它将通常的函数用泛函来代替,泛函就是从一个函数空间到 $\mathbb{R}$ 或 $\mathbb{C}$ 的映射,但是他和他的后继者缺少了以后才出现的一些代数和拓扑的工具来发展它们。近代分析的产生伴随着"无穷代数"的进展,"无穷代数"是和经典的线性代数密切相关联的,后者到了 1890 年(直到对偶的概念,这是以后才有的)已经扎实地建立起来了。强烈地受到代数方法的启示,Fredholm 在 19 世纪时的工作中出现了一个算子的核概念,这成为了近代积分方程理论的一个基石。Hilbert 对于对称核比 Fredholm 又进了一步,他揭示了与实二次型理论的类似性,从而使得平方可积函数这一概念的重要性清晰了。有了 Hilbert 的工作:积分方程一般理论之基础(*Grundzüge einer allgemeinen Theorie der Integralgleichung*),就跨出了从"无穷的代数"到"无穷几何"的一步。Fréchet 的贡献则在于引入了带有距离的空间的抽象概念,从而使得从 Euclid 几何转向从那时起就称之为 Hilbert 空间的框架成为可能,Hilbert 空间是数学和量子物理学的一个基本概念。

泛函分析在量子系统研究中的有用性是在 20 世纪 50 年代明确的,当时 Kato 证明了原子的 Hamilton 量的自共轭性,以及 Garding 和 Wightman 刻画了量子场理论中的公理。从此泛函分析就与量子场理论许多方面的核心相联系了。泛函分析的应用扩展到了数学的许多分支,其中有数值分析、整体分析、伪微分算子理论、微分几何、算子代数、非交换几何等。

拓扑向量空间

人们遇到的拓扑空间最多的实际上是距离空间。拓扑空间 E 上的一个距离是一个映射 $d:E\times E\to[o,\infty[$,它是对称的,使得 $d(u,v)=0\Leftrightarrow u=v$ 并满足三角不等式 $d(u,w)\leqslant d(u,v)+d(v,w)$ 对所有的向量 u,v,w 成立。一个拓扑空间 E 是可距离化的,如果 E 上有一个距离 d 和 E 上的拓扑相容,这时以任意点 $x\in E$ 为心,以 $1/n$ 为半径的球构成了 x 处的局部基——就是说:x 的一组邻域使得 x 的每个邻域都包含这一组中的一个元。E 中的序列 (u_n) 收敛于 $u\in E$ 当且仅当 $d(u_n,u)$ 收敛于 0。

在完备距离空间 (E,d) 上的 Banach 不动点定理是非线性泛函分析中的一个有用工具:它表明 E 上的一个(严格)压缩,就是,有固定的 $\sigma<k<1$ 使得映射 $T:E\to E$ 满足 d

$(Tu,Tv)\leqslant k\mathrm{d}(u,v)$[①]对所有 $u\neq v\in E$ 成立,那么它有惟一的不动点 $Tu_0=u_0$。特别地,对微分方程 $\mathrm{d}y/\mathrm{d}t=F(y,t)$,其初始条件 $y(0)=y_0$,而 F 是 Lipschitz 连续的,它提供了解的局部存在性和惟一性。

线性泛函分析起始于拓扑向量空间,就是一个向量空间赋予了一个拓扑,对这个拓扑其(线性结构的)运算是连续的。一个拓扑向量空间赋予了一个局部基,它的元是凸的,就称之为局部凸的。局部凸空间的例子是赋范线性空间,即向量空间赋予了一个范数,这个概念首次出现在 Fréchet 的工作中。向量空间 V 上的一个半范数是一个映射 $\rho:V\to[o,\infty[$,它服从三角不等式 $\rho(u+v)\leqslant\rho(u)+\rho(v)$对所有的 u,v 成立,并且对任意的标量 λ 和向量 u 有$\rho(\lambda u)=|\lambda|\rho(u)$;如果还有 $\rho(u)=0\Rightarrow u=0$,它是一个范数,经常记作$\|\cdot\|$。向量空间上的范数带出了一个平移不变的距离函数 $\mathrm{d}(u,v)=\|u-v\|$,使之成为一个距离空间。

历史上最早的赋范空间例子之一是 $C([0,1])$空间,它是 Riesz 所讨论的区间$[0,1]$上的(实值或复值)连续函数空间,赋以最大值范数$\|f\|_\infty:=\sup_{x\in[0,1]}|f(x)|$。20 世纪 20 年代,伴随着 Hahn 和 Banach 的工作产生了 Banach 空间的一般定义。一个赋范线性空间是一个 Banach 空间,如果作为一个由它诱导出的距离的距离空间是完备的,$C([0,1])$是一个典型的 Banach 空间。更为一般的,对任意非负整数 k,$[0,1]$上的 C^k 类函数空间$C^k([0,1])$,赋予范数 $\|f\|_k=\sum_{i=0}^k\|f^{(i)}\|_\infty$,即被表示成有限个半范数$\|f^{(i)}\|_\infty=\sup_{x\in[0,1]}|f^{(i)}x|$,$i=0,\cdots,k$ 的项之和,它也是 Banach 空间。

区间$[0,1]$上的光滑函数空间 $C^\infty([0,1])$就不再是 Banach 空间,这是由于它的拓扑是由可数个半范数族$\|f\|_k$ 所刻画的,其中 k 在正整数范围内变化。距离

$$\mathrm{d}(f,g)=\sum_{k=1}^{\infty}2^{-k}\frac{\|f-g\|_k}{1+\|f-g\|_k}$$

使得它成为了一个 Fréchet 空间,就是一个局部凸的完备距离空间。对速降函数空间 $\mathcal{S}(\mathbb{R}^n)$,其元素速降函数是 $\mathbb{R}^n$ 上的光滑函数 f 并且

$$\|f\|_{\alpha,\beta}:=\sup_{x\in\mathbb{R}^n}|x^\alpha D_x^\beta f(x)|$$

对每个多重指标 α 和 β 都是有穷的,$\mathcal{S}(\mathbb{R}^n)$也是 Fréchet 空间,它的拓扑是由半范数$\|\cdot\|_{\alpha,\beta}$给定的。Fréchet 空间除此之外的例子是具有一个固定的紧支集 $K\subset\mathbb{R}^n$ 的光滑函数空间 $C_o^\infty(K)$,赋以可数的半范数

$$\|D^\alpha f\|_{\infty,K}=\sup_{x\in K}|D_x^\alpha f(x)|,\alpha\in\mathbb{N}_0^n$$

另一个空间是一个闭流形 M 上的向量丛 E 的光滑截面空间 $C^\infty(M,E)$,赋予一个类似的可数半范数族。给定一个开子集 $\Omega=\bigcup_{p\in\mathbb{N}}K_p$,其中 $K_p(p\in\mathbb{N})$是 $\mathbb{R}^n$ 的紧子集,赋予空间 $\mathcal{D}(\Omega)=\bigcup_{p\in\mathbb{N}}C_o^\infty(K_p)$归纳极限拓扑——$\mathcal{D}(\Omega)$中的序列$(f_n)$收敛到 $f\in\mathcal{D}(\Omega)$,如果每个 f_n 的支集在某个固定的紧子集 K 中并且对每个多重指标 α,$(D^\alpha f_n)$在 K 上一致收敛于 $D^\alpha f$——$D(\Omega)$是一个局部凸空间。

Banach 空间中的 Hilbert 空间具有和有穷维空间很相似的性质,它在历史上是在 20 世纪初出现在 Hilbert 工作中的第一类无穷维空间。一个 Hilbert 空间是一个 Banach 空

① 原文此处有误——译者注。

间,它有一个从内积导出的范数$\|\cdot\|$,就是$\|u\|^2=\langle u,u\rangle$,$\langle\cdot,\cdot\rangle$是一个正定的双线性(或共轭双线性,这要根据基空间是实的还是复的来确定)型。Hilbert 空间是量子力学结构的基本成分;使用(闭的)张量乘积,人们从一个 Hilbert 空间 H 出发构造出 Fock 空间 $\mathcal{F}(H)=\sum_{k=0}^{\infty}\otimes^k H$,和玻色子 Fock 空间 $\mathcal{F}(H)=\sum_{k=0}^{\infty}\otimes_s^k H$(其中$\otimes_s$是(闭的)对称化的张量乘积)以及费米子 Fock 空间 $\mathcal{F}(H)=\sum_{k=0}^{\infty}\Lambda^k H$(这里 Λ^k 是反对称化的(闭)张量乘积)。

一个典型的 Hilbert 空间是使得 $\sum_{n\in\mathbb{Z}}|u_n|^2$ 有穷的复值序列$(u_n)_{n\in\mathbb{Z}}$的空间 $l_2(\mathbb{Z})$,这个空间已经暗含在 Hilbert 的工作"基础"(Grundzügen)中了。这之后很快,借助于 Lebesgue 引入的积分工具,Riesz 和 Rischer 证明了区间$]0,1[$上的平方可和函数,也就是满足

$$\|f\|_{L^2}=\left(\int_0^1|f(x)^2|\,\mathrm{d}x\right)^{1/2}$$

为有穷的函数 f,构成的空间 $L^2(]0,1[)$(首次由 Riesz 所引入)是 Hilbert 空间。这些又进一步推广到$]0,1[$上的 p 一次可和($1\leqslant p<\infty$)函数(即那些满足

$$\|f\|_{L^p}=\left(\int_0^1|f(x)|^p\mathrm{d}x\right)^{1/p}$$

为有穷的函数 f)空间 $L^p(]0,1[)$,除了 $p=2$ 它们不是 Hilber 空间,但却提供了 Banach 空间的另一些例子,$]0,1[$上的按 Lebesgue 测度几乎处处有界的函数空间 $L^\infty(]0,1[)$则是 Banach 空间的另一个例子。

1936 年,Sobolev 用分部积分的方法推广了函数和它们的导数的概念,这就引导出了所谓的 Sobolev 空间 $W^{k,p}(]0,1[)$,它包含的函数 $f\in L^p(]0,1[)$且直到 k 阶的导数也在 $L^p(]0,1[)$中,空间是作为 $C^\infty(]0,1[)$,以

$$f\longmapsto\|f\|W^{k,p}=\left(\sum_{j=0}^{k}\|\partial^j f\|_{L^p}^p\right)^{1/p}$$

为范数取得的闭包($p=2$ 时,$W^{k,p}(]0,1[)$是 Hilbert 空间,通常记成 $H^k(]0,1[)$。空间 $W^{k,p}(]0,1[)$不同于 Sobolev 空间 $W_0^{k,p}(]0,1[)$,与它相对应的是集合 $D(]0,1[)$对于范数 $f\to\|f\|W^{k,p}$的闭包;例如 $u\in W^{1,p}(]0,1[)$是 $W_0^{1,p}(]0,1[)$中的元当且仅当它在 0 和 1 处为零,即它在区间的边界上满足 Dirichlet 型边界条件。类似地,我们可以空义 $\mathbb{R}$ 上的 Sobolev 空间 $W_0^{k,p}(\mathbb{R})=W^{k,p}(\mathbb{R})$,开子集 $\Omega\subset\mathbb{R}^n$ 上的 Sobolev 空间 $W^{k,p}(\Omega)$和 $W_0^{k,p}(\Omega)$,以及在一个闭流型 M 上使用单位分解以定义 M 上向量丛 E 截面的 Sobolev 空间 $H^k(M,E)=W^{k,2}(M,E)$。用傅里叶变换(以后讨论),我们可以去掉 k 是一个整数的假设,从而把 Sobolev 空间的概念扩充到定义 $W^{s,p}(\Omega)$和 $H^s(M,E)$,其中 s 是任意实数。

Sobolev 空间出现在许多数学领域;概率理论的一个重要的例子是 Cameron-Martin 空间 $H^1(]0,t[)$,它嵌入到 Wiener 空间 $C([0,t])$中。这个嵌入是更为一般的 Sobolev 嵌入定理的一个特例,定理将 Sobolev 空间 $W^{k,p}$嵌入到(可能是连续的,有时甚至是紧的(紧算子的概念将在以后的章节中讨论))空间 L^q 中,这里 $q>p$,且有这样的连续包含关系 $W^{k,p}(\mathbb{R}^n)\subset L^q(\mathbb{R}^n)$,其中 $1/q=1/p-k/n$,或者它包含在 C^l 空间中,$l\leqslant k$,即对于一个有界开并充分正规的 $\mathbb{R}^n$ 的子集 Ω 以及任意 $s\geqslant l+n/p$,$p>n$ 有连续包含关系 $W^{s,p}(\Omega)\subset C^l(\overline{\Omega})$(是 $C^l(\Omega)$中的函数的集合,$D^\alpha u$ 可以对所有的 $|\alpha|<l$ 连续地延拓到闭包 $\overline{\Omega}$ 上)。

Sobolev 嵌入定理在讨论偏微分方程解的正则性时有重要的应用,证明所得到的弱解实际上是光滑的。特别地,在一个 n 维的闭流形 M 上,如 $s>l+n/2$,则 Sobolev 空间 $H^s(M,E)$可以连续地嵌入到 C^l 类的 E 的截面空间 $C^l(M,E)$中,这就意味着超椭圆偏微分方程 $Au=v, v\in L^2(M,E)$的解是光滑的,例如 Seiberg-Witten 方程解。

对偶性

对偶性的概念(在拓扑的意义上)起始于 20 世纪之初的 Hadamard,他在寻找紧区间 I 上的连续函数赋以一致拓扑的 Banach 空间 $C(I)$上的连续线性泛函。它暗含在了 Hilbert 的理论之中,并且在 Riesz 的工作中是一个重要的部分,他设法将这个连续泛函表示成 Stieltjes 积分,这是近代积分理论的出发点之一。

一个拓扑向量空间 E 的拓扑对偶是 E 上的连续线性型组成的空间 E^*,当 E 是一个赋范空间时,连续线性型可以赋予对偶范数 $\|L\|_{E^*}=\sup_{u\in E,\|u\|\leqslant 1}|L(u)|$。

对偶空间经常带来新的格外的研究对象:任意一个函数 $f\in L^p(\mathbb{R}^n)(p\geqslant 1)$和在点 $x\in\mathbb{R}^n$ 的 δ 函数,$\delta_x: f\to f(x)$都在空间 $\mathcal{S}'(\mathbb{R}^n)$中,它是与 $\mathcal{S}(\mathbb{R}^n)$对偶的 $\mathbb{R}^n$ 上的缓增分布,它自身包含在与 $\mathcal{D}(\mathbb{R}^n)$对偶的分布空间 $\mathcal{D}'(\mathbb{R}^n)$中。进而,核空间 E 的拓扑对偶 E^* 包含有一个概率测度的支集,它具有由一个 E 上的连续正定函数给出的特征函数(见下一节)。核空间中的投影极限是 $E=\bigcap_{p\in\mathbb{N}}H_p$(一个序列$(u_n)\in E$ 收敛于 $u\in E$ 只要在每个 H_p 中都收敛于 u),这里可数多个 Hilbert 空间的网$\cdots\subset H_p\subset_{H_{p-1}}\subset\cdots\subset H_o$,使得嵌入 $H_p\subset H_{p-1}$是一个迹类算子(见"算子代数"一节)。如果 H_p 是 E 对于范数$\|\cdot\|_p$ 的闭包,E 拓扑对偶 E'是一个归纳极限 $E'=\bigcup_{p\in\mathbb{N}_o}H_{-p}$,这里 H_{-p}是(H_p 的)对偶 Hilbert 空间以$\|\cdot\|_{-p}$为范数(E'中的序列(u_n)收敛于 $u\in E'$只要它在某个 H_{-p}中且按 H_{-p}的拓扑收敛于 u),我们有

$$E\subset\cdots\subset H_p\subset H_{p-1}\subset\cdots\subset H_o$$
$$=H_o'\subset H_{-1}\subset\cdots\subset H_{-p}\subset\cdots\subset E'$$

一个闭流形上的椭圆算子理论的一个结果是:一个闭流形 M 上的向量丛的光滑截面 Fréchet 空间 $C^\infty(M,E)$是核的,它可数多个 Sobolev 空间 $H^p(M,E)$的投影极限,而它的对偶由可数多个 Sobolev 空间 $H^{-p}(M,E)$的归纳极限给出①。

一个赋范线性空间 E 上非零的连续线性型的存在性是由 Hahn-Banach 定理予以确定的,该定理说*对 E 的任意闭的线性子空间 F,存在一个非零的连续线性型,它在 F 上为零*。当空间是一个 Hilbert 空间$(H,\langle\cdot,\cdot\rangle_H)$时,从 Riesz-Fréchet 定理得出,$H$ 上的任一连续线性型 L 都可以惟一地用一个向量 $v\in H$ 来表示,使得 $L(u)=\langle v,u\rangle_H$ 对所有的 u 成立,这样偶对的左方和右方作 Hilbert 内积,从而将拓扑对偶 H^* 等同于了 H。

在一个赋范向量空间上由范数导出的强拓扑——在这个拓扑下,序列(u_n)收敛于 u 是指$\|u_n-u\|\to 0$——在 E 是无穷维的情形,这对于紧集它是太过细了,因为对于强拓扑单位球的紧性是有穷维空间的特性。由于紧集在存在性定理中是有用的,人们有意弱化拓扑:E 上的弱拓扑——它在 E 是有穷维的情形是和强拓扑一致的,在弱拓扑下一个序列(u_n)收敛于 u 当且仅当 $L(u_n)\to L(u)\ \forall L\in E^*$——下单位球是紧的当且仅当 E 是自

① 该段中原文有一些错误,已做了改正,不在此一一列举——译者注。

反的,换言之,E 能典则地等同于它的二次对偶$(E^*)^*$。对于 $1<p<\infty$,给定一个开子集 $\Omega\subset\mathbb{R}^n$,$L^p(\Omega)$的拓扑对偶借助于 Riesz 表示能等同于 $L^{p^*}(\Omega)$,这里 p^* 共轭于 p,即 $1/p+1/p^*=1$ 并且 $L^p(\Omega)$是自反的,然而 $W^{s,p}(\Omega)$和 $W_0^{s,p}(\Omega)$的拓扑对偶两者都是 $W_0^{-s,p^*}(\Omega)$,所以只有 $W_0^{s,p}(\Omega)$是自反的。$L^1(\Omega)$和它的拓扑对偶 $L^\infty(\Omega)$都不是自反的,因为 $L^1(\Omega)$严格地包含在 $L^\infty(\Omega)$的拓扑对偶中,有 $L^\infty(\Omega)$上的连续线性型 L 它不具有如下的形式

$$L(u)=\int_\Omega uv,\forall u\in L^\infty(\Omega),\text{这里 } v\in L^1(\Omega)$$

类似地,一个赋范线性空间 E 的拓扑对偶 E^* 可以赋予由对偶范数$\|\cdot\|_{E^*}$ 导出的拓扑和弱* 拓扑,后者是使得映射 $L\longmapsto L(u),u\in E$ 是连续的最弱的拓扑,在这个拓扑下 E^* 中的单位球是紧的(Banach-Alaoglu 定理)。

对偶性并不总能保留可分性——一个拓扑向量空间是可分的如果它有一个可数稠子空间—— $L^\infty(\Omega)$空间不是可分的,它是 $L^1(\Omega)$的拓扑对偶,而 $L^1(\Omega)$是可分的。然而 Hahn-Banach 定理的结论是:如果一个 Banach 空间的拓扑对偶是可分的,那么原空间也是,如果再加上自反的假设条件那么就一致了;一个 Banach 空间是自反和可分的只要它的拓扑对偶是就行了。对于 $1\leqslant p<\infty$,$L^p(\Omega)$和 $W_0^{s,p}(\Omega)$是可分的,如果 $p\neq1$ 还是自反的。

傅里叶变换

在 18 世纪中叶,Bernouilli 把一根弦的振动解释成 n 个质点的振动当 n 趋于无穷时的极限情形,Bernouilli 引入了叠加原理的新概念,认为弦的振动可以分解成“固有振动”的叠加。这一观点引发了一场关于能否把一个任意函数展开成三角级数的讨论。另一个关于展开成“正交函数”(这一术语的使用始于 Hilbert)的例子也在那时出现在关于振动问题和热理论的讨论中,但只是在 19 世纪,有了傅里叶和 Dirichlet 的工作,叠加问题才得以解决。

可分的 Hilbert 空间提供了一组可数的正交系$\{e_n\}_{n\in\mathbb{Z}}$(对 H 上的标量积$\langle\cdot,\cdot\rangle_H$有$\langle e_n,e_m\rangle_H=\delta_{mn}$),它是完备的,就是每个向量 $u\in H$ 可以在这个系中惟一地展开成 $u=\sum_{n\in\mathbb{Z}}\hat{u}_n e_n$,它的傅里叶系数是 $\hat{u}_n=\langle u,e_n\rangle$。系数满足 Parseval 关系 $\sum_{n\in\mathbb{Z}}|\hat{u}_n|^2=\|u\|^2$(这里$\|\cdot\|$是和$\langle\cdot,\cdot\rangle$相关的范数),并且傅里叶变换 $u\longmapsto(\hat{u}(n))_{n\in\mathbb{Z}}$ 建立了可分 Hilbert 空间 H 和复数平方可和序列空间 $l^2(\mathbb{Z})$之间的一个等距同构。特别地,在单位圆 $S^1=\mathbb{R}/\mathbb{Z}$ 上具有通常 Haar 测度 $\mathrm{d}t$ 的 L^2 函数空间 $L^2(S^1)$是可分的,具有完备的正交系 $t\to e_n(t)=e^{2i\pi nt}$,$n\in\mathbb{Z}$,傅里叶变换

$$u\longmapsto\left(\hat{u}(n)=\int_0^1 \mathrm{e}^{-2i\pi nt}u(t)\mathrm{d}t\right)_{n\in\mathbb{Z}}$$

将该空间与空间 $l^2(\mathbb{Z})$等同了起来。在这一等同下投影 $p_+:u\longmapsto(u_n)_{n\in\mathbb{N}}$ 在 $l^2(\mathbb{Z})$中的值域,所得到的 Hilbert 空间 $l^2(\mathbb{N})$就相应于 Hardy 空间 $\mathcal{H}^2(S^1)$。

傅里叶变换扩展到了空间 $S(\mathbb{R}^n)$,取 $f\in\mathcal{S}(\mathbb{R}^n)$,映射

$$f\longmapsto\hat{f}(\xi)=\frac{1}{\sqrt{(2\pi)^n}}\int_{\mathbb{R}^n}\mathrm{e}^{-i\xi\cdot x}f(x)\mathrm{d}x$$

将 $\mathcal{S}(\mathbb{R}^n)$线性连续地映到它自身之上,它有连续逆 $f \longmapsto \hat{f}(-\xi)$。$n=1$ 时,泊松公式建立了 $f\in\mathcal{S}(\mathbb{R})$和它的傅里叶变换 $\hat{f}$ 之间的关系 $\sum_{n=-\infty}^{\infty} f(2\pi n) = \sum_{n=-\infty}^{\infty} \hat{f}(n)$。

傅里叶变换将对一个多重指标 $\alpha=(a_1,\cdots,a_n)$的微分运算 D_ξ^α转换(直到差一个乘常数因子)成对 $\xi^\alpha=\xi_1^{a_1}\cdots\xi_n^{a_n}$ 的乘法,所以可以用来定义 Sobolev 空间 $W^{s,p}$,其中 s 是一个实数,这是一个具有有穷 Sobolev 范数 $\|u\|_{W^{s,p}} = \left(\int |(I+|\xi|^s\hat{u})(\xi)|^p\right)^{1/p}$ 的 L^p 函数空间(它和先前定义的当 $s=k$ 是一个非负整数的情形是一致的)。

傅里叶变换还用来描述一个线性伪微分算子 A(见下面两个章节要讨论的有界和无界线性算子的概念),A 是 a 阶的是依据它的符号 σ_A 作用在 $\mathbb{R}^n$ 的开子集上的光滑函数上——σ 是 $U\times\mathbb{R}^n$ 的一个光滑映射在 x 中有紧支集,对任意的多重指标 $\alpha,\beta\in\mathbb{N}_0^n$ 有常数 $C_{\alpha,\beta}$满足

$$|D_x^\alpha D_\xi^\beta \sigma(x,\xi)| \leqslant C_{\alpha,\beta}(1+|\xi|)^{\alpha-|\beta|}$$

对一切 $\xi\in R^n$ 成立——且有

$$(Af)(x) = \frac{1}{\sqrt{(2\pi)}^n}\int_{R^n} e^{-ix\cdot\xi}\sigma_A(x,\xi)\hat{f}(\xi)d\xi$$

傅里叶变换将一个 $\mathbb{R}^n$ 上的高斯函数 $x \longmapsto e^{-(1/2)\lambda|x|^2}$($\lambda$ 是一个非零标量)映成另一个高斯函数 $\xi \longmapsto e^{-(1/2)\lambda^{-1}|\xi|^2}$(直到差一个非零乘法因子),这是弦理论中的 T-对偶性的一个出发点。更为一般的,一个 Hilbert 空间 H 上的具有协方差 C 的高斯概率测度 μ 的特征函数

$$\hat{\mu}(\xi) := \int_H e^{i(x,\xi)_H}\mu(dx)$$

是函数 $\xi \longmapsto e^{-(1/2)(\xi\cdot C\xi)_H}$。这样的概率测度在 Euclidean 量子场理论中是典型的;在公理化量子场理论中,n 点函数的解析性质可以用傅里叶变换从 Wightman 公理中推导出来。这样傅里叶变换成了量子场理论诸多不同方面的基础。

Fredholm 算子

一个[0,1]×[0,1]上的复值连续函数 K 产生了一个[0,1]上复值连续函数(赋以极大值范数$\|\cdot\|_\infty$)的积分算子

$$A: f \to \int_0^1 K(x,y)f(y)dy$$

它有如下的上界性质

$$\|Af\|_\infty \leqslant \mathrm{Sup}_{[0,1]\times[0,1]}|K(x,y)|\,\|f\|_\infty$$

换言之,A 是一个有界线性算子,范数以 $\mathrm{Sup}_{[0,1]\times[0,1]}|K(x,y)|$ 为上界;一个从赋范线性空间$(E,\|\cdot\|_E)$到另一个赋范线性空间$(F,\|\cdot\|_F)$的线性算子 $A:E\to F$ 是有界的(或连续的)当且仅当(算子)范数$|\|A\||:=\mathrm{Sup}\|u\|_{E\leqslant 1}\|Au\|_F$ 是有界的。

一个用连续核 K 定义的积分算子

$$A: f \to \int_0^1 K(x,y)f(y)dy$$

还是紧的;一个紧算子是一个赋范空间的有界算子并且将有界集合映射成一个预紧集合,

即集合的闭包是紧的。赋范空间上紧算子的另一些例子是有穷秩算子,这些算子有有穷维的值域。事实上,一个可分 Hilbert 空间上的任意的紧算子都可以用一个有穷秩算子的序列以算子范数$\|\|\cdot\|\|$导出的拓扑来逼近。

在上面提到的积分算子的情形,Volterra 提出方程 $f=(1-A)\phi, f\in C([0,1])$的连续解是 $\phi=(1-A)^{-1}f$,受到这个工作的启发,Fredholm 在 1900 年的"论一类泛函方程"(*Sur une class déquation functionnlles*)中引入了一个复参数 λ,讨论方程 $f=(1-\lambda A)\phi$。他证明了从那时起称之为 Fredholm 的备择,它表明或者方程 $f=(1-\lambda A)\phi$ 对每一个$f\in C([0,1])$有惟一解,或者齐次方程$(I-\lambda A)\phi=0$ 有非零解。用现在的话来讲,这意味着一个紧线性算子 A 的预解式 $R(A,\mu)=(A-\mu I)^{-1}$ 是满射的充要条件是它是单射的。Fredholm 的备择定理是解偏微分方程的强有力工具,在这些方程中有 Dirichlet 问题,它的解是在某个区域 $\Omega\subset\mathbb{R}^n$ 上的调和函数 u(即 $\Delta u=0$,这里 $\Delta=-\sum_{i=1}^{n}\partial^2/\partial x_i^2$),$u$ 还要满足 Dirichlet 边界条件 $u|_{\partial\Omega}=f$,这里 f 是边界$\partial\Omega$ 上的连续函数。Dirichlet 问题有几何上的应用,特别是对于非线性 Plateau 问题,它是在给定边界曲线的条件下求在 $\mathbb{R}^d$ 中的最小表面积,它化成了一个(线性)Dirichlet 问题。

从紧算子 A 构造出算子 $B=I-A$,它是一个特殊的 Fredholm 算子,Fredholm 算子是有界线性算子 $B:E\to F$,它"差一个紧算子"是可逆的,就是存在一个有界线性算子 $C:F\to E$,使得 $BC-I_F$ 和 $CB-I_E$ 两者紧。一个 Fredholm 算子 B 有一个穷维的核 $\ker B$,当$(E,\langle\cdot,\cdot\rangle_E)$和$(F,\langle\cdot,\cdot\rangle_F)$是 Hilbert 空间时算子 B 的余核 $\mathrm{Ker}\,B^*$ 也是有穷维的,这里 B^* 是 B 的共轭它定义成

$$\langle Bu,v\rangle_F=\langle u,B^*v\rangle_E \qquad \forall u\in E,\forall v\in F,$$

所以就有了算子指标的定义 $\mathrm{ind}(B)=\dim(\mathrm{Ker}\,B)-\dim(\mathrm{Ker}\,B^*)$,这是指标理论的一个出发点。Töplitz 算子 T_ϕ,这里 ϕ 是单位圆上的一个连续函数,提供了 Fredholm 算子的第一个例子;它作用在 Hardy 空间 $\mathcal{H}^2(S^1)$上:

$$Te_{-n}\Big(\sum_{m\geqslant 0}a_m e_m\Big)=\sum_{m\geqslant 0}a_{m+n}e_m$$

这里有等同关系 $\mathcal{H}^2(S^1)\simeq l^2(\mathbb{N})\subset l^2(\mathbb{Z})$,$l^2(\mathbb{Z})$赋予正则完备的正交基$(e_n,n\in\mathbb{Z})$。Fredholm 指标 $\mathrm{ind}(T_{e_{-n}})$是正整数 n,所以它的共轭的指标是$-n$,由此得出结论 Fredholm 算子的指标映射是到整数映上的。

单参数(半)群

与有穷维的情形不同,两个赋范线性空间$(E,\|\cdot\|_E)$和$(F,\|\cdot\|_F)$之间的一个线性算子 $A:E\to F$ 不能期望它是有界的。在偏微分方程中出现的无界算子包括象在开子集 $\Omega\subset\mathbb{R}^n$ 上的拉普拉斯算子 Δ。以下举出偏微分方程一些基本的例子,它们出现在泊松、傅里叶和柯西研究数学物理各种问题的辛劳工作中:

$$\Delta u=0 \qquad \text{拉普拉斯方程}$$

$$\frac{\partial^2 u}{\partial t^2}+\Delta u=0 \qquad \text{波动方程}$$

$$\frac{\partial u}{\partial t}+\Delta u=0 \qquad \text{热传导方程}$$

以及以后量子力学中的 Schrödinger 方程:

$$i\frac{\partial u}{\partial t}=\Delta u$$

这里 t 是时间参数。

一个无穷维赋范空间上的一个无界线性算子通常定义在一个区域 $D(A)$ 上,它是严格包含在 E 中的。拉普拉斯算子 Δ 就是定义在 $L^2(\mathbb{R}^n)$ 中的稠定义域 $D(A)=H^2(\mathbb{R}^n)$ 上;它定义了一个从 $H^2(\mathbb{R}^n)$ 到 $L^2(\mathbb{R}^n)$ 的有界算子,但不能延拓成为 $L^2(\mathbb{R}^n)$ 上的一个有界算子。跟这个算子一样,我们所遇到的绝大多数无界算子 $A:E\to F$ 在 E 中有稠密的定义域 $D(A)$ 并且是闭的,也就是它们的图像 $\{(u,Au),u\in D(A)\}$ 作为赋范线性空间 $E\times F$ 中的子集是闭的。在算子不是真的闭的情形,我们可以将它们闭化,就是说,进行闭延拓称之为算子的闭包。由闭图像定理,当 E 和 F 是 Banach 空间时,一个线性算子 $A:E\to F$ 是连续的只要它的图像是闭的,由此推出,定义在稠密定义域上的闭线性算子,如果它的定义域是全空间,是有界的。

对于一个有稠密定义域 $D(A)$ 的闭算子 $A:E\to F$,这里 E 和 F 是 Hilbert 空间,有内积 $\langle\cdot,\cdot\rangle_E$ 和 $\langle\cdot,\cdot\rangle_F$,$A$ 的共轭 A^* 在它的定义域 $D(A^*)$ 上定义成

$$\langle Au,v\rangle_F=\langle u,A^*v\rangle_E\quad\forall(u,v)\in D(A)\times D(A^*)$$

一个定义域是 $D(A)$ 的自共轭算子 A 是这样的:$D(A)=D(A^*)$ 和 $A=A^*$;$\mathbb{R}^n$ 上的拉普拉斯算子 Δ 是在 Sobolev 空间 $H^2(\mathbb{R}^n)$ 上自共轭的,但从根本上讲它只是在稠密定义域 $\mathcal{D}(\mathbb{R}^n)$ 上才是自共轭的,这意味着它的闭包是自共轭的。

无界自共轭算子能成为单参数有界算子半群的生成元。一个 Hilbert 空间 H 上的单参数有界算子族 $T_t,t\geqslant 0(T_t,t\in\mathbb{R})$ 是一个半群(群)如果满足 $T_sT_t=T_{t+s}\ \forall t,s\geqslant 0(\forall t,s\in\mathbb{R})$ 和它是强连续的(或简称为连续):对任意 $t_0\geqslant 0(t_0\in\mathbb{R})$ 和 $u\in H$ 有 $\lim\limits_{t\to t_0}T_tu=T_{t_0}u$。

Stone 定理建立起了 Hilbert 空间上连续单参数酉($U_t^*U_t=U_tU_t^*=I$)群 $U_t,t\in\mathbb{R}$ 且 $U_0=\mathrm{Id}$,和自共轭算子 A 之间的一一对应,从 $U_t,t\in\mathbb{R}$ 得到群的无穷小生成元:iA[①]

$$iAu=\lim_{t\to 0}\frac{U_tu-u}{t},\quad u\in D(A)$$

所以可以紧凑地写成 $U_t=\mathrm{e}^{itA}$。量子力学中的一个重要的例子是 $U_t=\mathrm{e}^{itH}U_0,t\in\mathbb{R}$,$H$ 是自共轭的 Hamilton 量,它是 Schrödinger 方程 $\mathrm{d}u/\mathrm{d}t=iHu$ 的解。Lie-Trotter 公式,它对于 Feynman 的路径积分有重要的应用,表示出了由 $A+B$ 生成的酉群,其中 A,B 和 $A+B$ 都是在它们各自定义域上的自共轭算子,酉群表示成了一个强极限

$$\mathrm{e}^{it(A+B)}=\lim_{n\to\infty}(\mathrm{e}^{\frac{itA}{n}}\mathrm{e}^{\frac{itB}{n}})^n$$

另一方面,Hilbert 空间 $(H,\langle\cdot,\cdot\rangle_H)$ 上的正定算子——就是 A 是自共轭的且 $\langle Au,u\rangle_H\geqslant 0,\forall u\in D(A)$——生成了单参数半群 $T_t=\mathrm{e}^{-tA},t\geqslant 0$。Hille 和 Yosida 证明了在一个 Hilbert 空间上,强连续压缩(即 $\|T_t\|\leqslant 1,\forall t\geqslant 0$)半群且 $T_0=\mathrm{Id}$ 是一一对应于稠定的正定算子 $A:D(A)\subset H\to H$,它是极大的(即 $I+A$ 是映上的),无穷小生成元可以从相应的半群得出

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① 原文此处有误 ——译者注。

$$-Au=\lim_{t\to 0}\frac{T_t u-u}{t},u\in D(A)$$

类似地,一个 Hilber 空间上的正稠定的自共轭算子 A 产生了一个稠定闭对称共轭双线性型$(u,v)\longmapsto(\sqrt{A}u,\sqrt{A}v)$(见下一节$\sqrt{A}$的定义;$\langle\cdot,\cdot\rangle_H$ 是 H 上的内积),并且这一映射产生了算子和具有前述性质的共轭双线型之间的一一对联应,这是 Dirichlet 型理论的出发点之一。对于一个可分的 Banach 空间 E 上的概率测度 μ,我们可以将它与一个 Hilbert 空间 $H,E^*\subset H^*=H\subset E$,上的一个稠定闭对称共轭双线性型(事实上是一个 Dirichlet 型)相关联,这是 Wiener 空间 $E=C([0,t])$ 上标准的 Wiener 测度 μ 和由 Cameron-Martin 空间 $H=H^1([0,t])$给出的 Hilbert 空间的特殊情形,双线性型是

$$(u,v)\longmapsto\int\langle\bar{\nabla}u,\bar{\nabla}v\rangle_H$$

这里$\bar{\nabla}$是闭 Malliavin 梯度。

Δ 是 $\mathbb{R}^n$ 上的拉普拉斯算子,$-\Delta$ 生成了热算子半群 $e^{-t\Delta}$,$t\geqslant 0$。它有一个光滑的核 $K_t\in C^\infty(\mathbb{R}^n\times\mathbb{R}^n)$,定义是

$$(e^{-t\Delta}f)(x)=\int_{\mathbb{R}^n}K_t(x,y)f(y)\mathrm{d}y,\quad\forall f\in C_0^\infty(\mathbb{R}^n)$$

这是一个光滑算子,将 Sobolev 函数映成光滑函数的算子。一般地,一个 $\mathbb{R}^n$ 的开子集 U 上具有符号 σ_A 的一个伪微分算子 A 只能有一个分布的核

$$K_A(x,y)=\int_{\mathbb{R}^n}e^{i\langle x-y,\xi\rangle}\sigma(\xi)\mathrm{d}\xi$$

$\mathbb{R}^n$ 上的拉普拉斯算子的逆$(\Delta+m^2)^{-1}$的核(非负实数 m^2 表示质量)称之为 $\mathbb{R}^n$ 上的 Green 函数,它在 Feynman 图像理论中起了根本性的作用。

谱理论

谱理论研究的是复参数 λ 的值分布,这些 λ 使得对给定的赋范空间 E 上的一个线性算子 A,算子 $A-\lambda I$ 有逆,以及如果逆存在,这个逆就是算子 A 的预解式 $R(A,\lambda)=(A-\lambda I)^{-1}$的性质。$A$ 的谱集 $\mathrm{Sp}(A)$是 A 的预解集在 C 中的补;它是 3 个不相交集合的并;使得 $A-\lambda I$ 不是单射的所有复数λ 的集合称之为点谱——这样的 λ 是 A 的本征值,有相应的本征函数 $u\in D(A)$,$Au=\lambda u$;使得 $A-\lambda I$ 有一个稠定的无界逆 $R(A,\lambda)$的 λ 的集合,称之为连续谱;以及使 $A-\lambda I$ 有一个无界但不稠定的逆 $R(A,\lambda)$的 λ 组成剩余谱。

一个有界算子的谱集是有界的;作用在一个 Hilbert 空间上的自共轭算子 A 有实谱集且没有剩余谱,因为 $A-\lambda I$ 的值域是稠的。作为 Fredholm 备择定理的一个结果,紧算子的谱集中只有点谱;它是可数的以 0 为聚点。量子力学系统的一个 Hamilton 量的点谱和连续谱两者都有,其中的点谱特别有意义因为与之对应的本征函数是系统的稳态。正如 Kac 首次所指出的(你能听得出鼓的形状吗?),作用在函数上的一个算子的谱能够反映出这些函数所在的空间的几何,这是在微分几何中许多有趣并影响深远的问题的出发点。

一个 Hilbert 空间上的一个自共轭线性算子可以用一簇投影 $E_\lambda(\lambda\in\mathbb{R})$加以刻划,这就是谱表示

$$A=\int_{\mathrm{Sp}(A)}\lambda\mathrm{d}E_\lambda$$

给出$\mathbb{R}$上的一个 Borel 实值函数 f,算子

$$f(A)=\int_{\mathrm{Sp}(A)} f(\lambda)\mathrm{d}E_\lambda$$

是另一个自共轭算子。某个 Hilbert 空间$(H,\langle\cdot,\cdot\rangle_H)$上一个具有稠定义域 $D(A)$的正算子 A 有非负的谱且对任意正实数 t,映射 $\lambda\longmapsto \mathrm{e}^{-t\lambda}$给出了相关联的有界热算子

$$\mathrm{e}^{-tA}=\int_{\mathrm{Sp}(A)} \mathrm{e}^{-t\lambda}\mathrm{d}E_\lambda$$

而映射 $\lambda\longmapsto\sqrt{\lambda}$则产生了一个正算子$\sqrt{A}$满足$\sqrt{A}^2=A$。预解式还可以用来从一个线性算子定义新的算子

$$f(A)=\frac{1}{2i\pi}\int_c f(\lambda)R(A,\lambda)\mathrm{d}\lambda$$

这就是沿着围绕谱的一个围道 C 的柯西型积分;用这种方法可以用来定义(本质自共轭的)正定的椭圆伪微分算子 A 的复数幂次A^{-z},并定义 A 的ζ函数$z\longmapsto\zeta(A,z)$。ζ函数是将普通的行列式扩展到了自共轭椭圆算子的ζ行列式的有用工具,从而对量子场理论的路径积分方法中的分割函数的意义提供了说明。

算子代数

一个 Hilbert 空间 H 上的有界线性算子组成了一个代数 $\mathcal{L}(H)$,它对于算子范数是闭的,并有由共轭运算 $A\longmapsto A^*$ 给出的对合;它还是 C^* 代数,即它是$\mathbb{C}$上的代数 A,有范数和对合 $*$,使得对这个范数 A 是闭的以及$\|ab\|\leqslant\|a\|\|b\|$和$\|a^*a\|=\|a\|^2$ 对所有$a,b\in A$成立,由 Gelfand-Naimark 定理,每个 C^* 代数同构于某个 $\mathcal{L}(H)$的子 C^* 代数。谱的概念从有界算子扩充到了 C^* 代数;一个 C^* 代数 A 中的一个元 a 的谱 $\mathrm{Sp}(a)$是复数 λ 的(紧)集合,这些 λ 使得 $a-\lambda\cdot 1$ 不可逆。自共轭的概念也扩展了$(a=a^*)$,并且如同自共轭算子 $B\in\mathcal{L}(H)$是非负的(在这个情形它的谱在 R^+ 中)当且仅当 $B=A^*A$ 对某个有界算子 A 成立一样,一个元 $b\in A$ 是非负的当且仅当对某个 $a\in A$ 有 $b=a^*a$,在这情形$\mathrm{Sp}(a)\subset\mathbb{R}_0^+$。

X 是某个局部紧的 Hausdorff 空间,连续函数 $f:\mathrm{X}\to\mathbb{C}$在无穷远处为零,这些 f 的代数 $C(\mathrm{X})$赋予极大范数以及复共轭 $f\longmapsto\bar{f}$ 后也是一个 C^* 代数,并且是一个典型的交换 C^* 代数,Gelfand 证明了如果 C^* 代数有单位元,则它等距同构于 $C(\mathrm{X})$),X 紧。对于一个 C^* 代数 A,我们可以与之关联到一个可交换群 $K_0(A)$,它是一个紧 Hausdorff 空间 X 上向量丛的同构类的 Grothendieck 群 $K^0(Z)$的对偶。

一个 Hilbert 空间上的紧算子构成了 C^* 代数 $\mathcal{L}(H)$的惟一真双边理想 $\mathcal{K}(H)$,它对于 $\mathcal{L}(H)$上的算子范数拓扑是闭的。Calkin 对一个可分 Hilbert 空间 H 的 $\mathcal{L}(H)$中的所有双边理想进行了分类,之后,商空间 $\mathcal{L}(H)/\mathcal{K}(H)$就称之为 Calkin 空间了;我们可以在这样的理想和一定的序列空间之间建立起一一对应。对应于复值序列(u_n)满足$\sum_{n\in N}|u_n|<\infty$的 Banach 空间 $l^1(\mathbb{Z})$的是迹类算子的 $*$ 理想 $\mathcal{I}_1(H)$。一个非负算子$A\in\mathcal{L}(H)$的迹 $\mathrm{tr}A=\sum_{n\in\mathbb{Z}}<Ae_n(e_n>_H)$ 在$[0,+\infty]$中,它不依赖于赋予 H 中内积$\langle\cdot,\cdot\rangle_H$ 的完备正交基$\{e_n,n\in\mathbb{Z}\}$的选取。$\mathcal{I}_1(H)$是满足$\|A\|_1=\mathrm{tr}(|A|)$为有界的 H

上的有界线性算子的 Banach 空间。给定一个(本质自共轭的)d 阶正微分算子 D,它作用在闭 n 维 Riemannian 流形 M 上的光滑函数上,它的复数幂次 D^{-z} 当 $\mathrm{Re}(z)>n/d$ 时是 M 上 L^2 函数空间上的一个迹类,并且相应的迹 $\mathrm{tr}(D^{-z})$ 扩展到整个平面上的一个半纯函数,ζ 函数 $\zeta(D,z)$ 在 0 点是全纯的。

更为一般地,满足 $\sum_{n\in\mathbb{Z}}|u_n|^p<\infty$ 的复数值序列 $(u_n)_{n\in\mathbb{Z}}$ 的 Banach 空间 $l^p(\mathbb{Z})$,$(1\leqslant p<\infty)$关联到 Schatten 理想 $\mathcal{I}_p(H)(1\leqslant p<\infty)$,这里的 $\mathcal{I}_p(H)$ 是满足 $\|A\|_p=(\mathrm{tr}|A|^p))^{1/p}$ 为有界的 H 上有界线性算子的 Banach 空间。正如所有的 l^p 序都收敛于 0,Schatten 理想 $\mathcal{I}_p(H)$ 都在 $\mathcal{K}(H)$ 中,我们有 $\cdots(\mathcal{I}_{p+1}(H))\subset\mathcal{I}_p(H)\subset\cdots\subset\mathcal{K}(H)$。

紧算子和 Schatten 理想在把指标理论扩展到非交换的情形时是有用的;一个对合代数 A 上的一个 Fredholm 模 (H,F) 是由一个 Hilbert 空间 H 中的 A 的一个对合表示 π 和 H 上一个满足 $F^2=\mathrm{Id}_H$ 的自共轭有界线性算子 F 所给出,而算子括号 $[F,\pi(a)]$ 对所有的 $a\in A$ 是紧的。对一个 p 可和的 Fredholm 模 (H,F),即对所有的 $a\in A$,$[F,\pi(a)]\in\mathcal{I}_p(H)$,我们可以相关联到由 A 上一个循环上闭链所给出的陈-特征 $\mathrm{ch}^*(H,F)$ 的一个表示 τ,它与 K 理论相配合以在 K 理论上建立一个整数值指标映射 τ。

Schatten 理想在讨论无穷维空间的几何时也是有用的,诸如环路群,对于它 Hilbert-Schmidt 算子($\mathcal{I}_2(H)$ 中的算子也称为 Hilbert-Schmidt 算子)是特别有用的。一个 Holder 型的不等式表明两个 Hilbert-Schmidt 算子的乘积是迹类。又进一步,对任意两个 Hilbert-Schmidt 算子 A 和 B,"循环性质"$\mathrm{tr}(AB)=\mathrm{tr}(BA)$ 成立,以及共轭双线性型 $(A,B)\longmapsto\mathrm{tr}(AB^*)$ 使 $\mathcal{L}_2(H)$ 成为一个 Hilbert 空间。

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导论:闵可夫斯基时空和狭义相对论

引言

闵可夫斯基时空通常被看作是能够把引力现象之外的其他物理定律进行公式化的一种适当的数学框架。在此,我们将用严格的术语来陈述这种数学框架,阐明那些已经被经验证明的事实,这些事实对闵可夫斯基时空做出了正确的物理解释,我们还要通过实例来描绘这种数学框架对于实现物理定律的公式化是合适的。

闵可夫斯基时空和洛伦兹群

闵可夫斯基时空 $\mathcal{M}$ 是一个四维实矢量空间,在其中定义了一个双线性形式 $g:\mathcal{M}\times\mathcal{M}\to R$,它是对称的(即对所有 $v,w\in\mathcal{M}$,有 $g(v,w)=g(w,v)$)并且是非退化的[对于所有的 $w\in\mathcal{M}$,$g(v,w)=0$ 意味着 $v=0$]。而且,g 具有 1 的指数,这就是说,在 $\mathcal{M}$ 中存在一组基矢$\{e_1,e_2,e_3,e_4\}$使得

$$g(e_a,e_b)=\eta_{ab}=\mathrm{diag}(1,1,1,-1)\ \text{其中}\ a,b=1,2,3,4$$

g 被称为 $\mathcal{M}$ 中的洛伦兹内积,而且这里给出的任何这种类型的基矢都是 $\mathcal{M}$ 中一组正交基矢。我们常把 g 在$(v,w)\in\mathcal{M}\times\mathcal{M}$ 上的值$g(v,w)$简写成 $v\cdot w$。如果矢量 v 的内积$v\cdot v$ 等于正的、负的或零,那么这个矢量就分别被称为类空矢量、类时矢量或零矢量(即类光矢量);所有零矢量的集合 C_N 被称为 M 中的零锥(即光锥)。如果$\{e_1,e_2,e_3,e_4\}$是一组正交基矢,而且定义 $v=v^1e_1+v^2e_2+v^3e_3+v^4e_4=v^ae_a$(这里使用了爱因斯坦的求和规则,即重复的上、下角标要对其所有的可能取值求和)以及 $w=w^be_b$,那么有

$$v\cdot w=v^1w^1+v^2w^2+v^3w^3-v^4w^4=\eta_{ab}v^aw^b$$

特别是,当且仅当

$$(v^4)^2=(v^1)^2+(v^2)^2+(v^3)^2$$

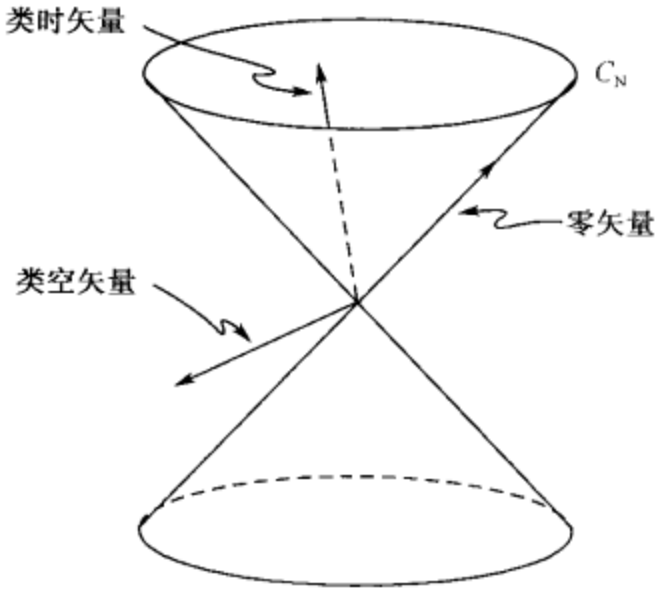

图 1　类空、类时和零矢量。

时,v 是零矢量(这里的零是指 C_N 的零“锥面”)。类时矢量位于这个零锥面的“内部”,类空矢量则位于零锥面的“外部”(见图 1)。

我们选取矢量空间 $\mathcal{M}$ 的某种取向,而且后面将始终只考虑 $\mathcal{M}$ 中的这种定向的正交基矢。从 $\mathbf{R}^3$ 的 Schwartz 不等式,我们可以看到(Naber 1992,定理 1.3.1),如果 v 是类时矢量,而 w 是非零的类时矢量或者类光矢量,那么当且仅当在任何正交基矢中满足 $v^4w^4>0$ 时,有 $v\cdot w<0$。特别是,当且仅当 $v\cdot w<0$ 时指定 v 和 w 这样两个矢量是等价的,那么就可以在所有类时矢量的集

合上定义一种等价关系。鉴于稍后将要看到的原因,我们可以说 v 和 w 具有相同的时间取向。存在两种等价的类型,一种类型是选择并指定指向将来。那么,另一种类型的类时矢量就被称为指向过去。我们可以看到(Naber 1992, 1.3 节及推论 1.4.5),这种分类也可以被推广到非零的零矢量(但是不能推广到类空矢量)。我们将把有确定指向的正交基矢称为时间指向的,如果它的类时矢量 e_4 指向未来;下面我们将只考虑这样的基矢。在 $\mathcal{M}$ 上的一个具有确定指向的、时间指向的和正交的基矢将被称为是一种可容许的基矢。如果 $\{e_1,e_2,e_3,e_4\}$ 和 $\{\hat{e}_1,\hat{e}_2,\hat{e}_3,\hat{e}_4\}$ 是两个那样的基矢,并且如果写成

$$e_b = \Lambda_b^1\hat{e}_1 + \Lambda_b^2\hat{e}_2 + \Lambda_b^3\hat{e}_3 + \Lambda_b^4\hat{e}_4 = \Lambda_b^a\hat{e}_a, \quad b=1,2,3,4 \qquad [1]$$

那么,可以显示矩阵 $\Lambda=(\Lambda_b^a)$ (a=行指标,b=列指标)满足下面 3 个条件(Naber 1992, 1.3 节):

(1)(正交性)$\Lambda^{\mathrm{T}}\eta\Lambda=\eta$, 其中 T 代表转置,$\eta=\mathrm{diag}(1,1,1,-1)$;

(2)(可定向性)$\det\Lambda=1$;

(3)(时间可定向性)$\Lambda_4^4\geqslant 1$。

我们将把任何一个满足上述 3 个条件的 4×4 矩阵 $\Lambda=(\Lambda_b^a)$ 称为洛伦兹变换(有时为了强调条件(2)和(3),会在前面分别添加上形容词"固有的"和"正交的")。这种矩阵的全体 L 在矩阵乘法下形成一个群,这个群就叫洛伦兹群。由正交性条件(1)很容易证明(Naber 1992, 引理 1.3.4),如果 $\Lambda_4^4=1$,那么 Λ 必须具有下面的形式:

$$\begin{pmatrix} & & & 0 \\ & (R_j^i) & & 0 \\ & & & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

其中 (R_j^i) 是 SO(3)群的一个元素,即一个具有行列式为 1 的 3×3 正交矩阵。这种形式的全部矩阵的集合 R 是洛伦兹群 L 的一个子群,称为转动子群。虽然对于我们现在所做的事情没有什么用处,但是还是应当指出,在很多应用中(例如,在粒子物理中)必须要考虑由洛伦兹群和时空平移($x^a\to x^a+\Lambda^a$,对于某些约束 Λ^a,$a=1,2,3,4$)在闵可夫斯基时空 $\mathcal{M}$ 中生成的更大的变换群,这个群被称为非齐次洛伦兹群,或者叫彭加勒群。

物理解释

要想说明在物理上如何想像闵可夫斯基时空和洛伦兹群,最好要(在直观上和术语上)把 $\mathcal{M}$ 中的"矢量"和 $\mathcal{M}$ 中的"点"(矢量的顶端)区分开来。$\mathcal{M}$ 中的点称为事件,虽然作为理想化的"点事件"没有空间尺度也没有时间的流逝,但是还是要把它想像成是真实发生的物理事件。例如,一种可能的物理图像是瞬时的碰撞,或者瞬时的爆炸,或者某种点粒子或光子(光的粒子)运动历程中的"瞬间"。

事件由坐标数值来确定。我们感兴趣的是由一个极特殊类型的观测者以一种特别的方式指定的事件坐标。特别是,我们能够容许的观察者全都处于三维右手笛卡儿空间坐标系,光子相对于这些坐标系在任何方向上都是沿直线运动。在坐标系的原点放有一只时钟,观察者可以通过所谓的斐索程序来确定真空中的光速 c(在时钟的读数是 t_1 的时刻从原点发射一个光子,然后由放置在 (x^1,x^2,x^3) 的一面镜子反射回来,原点的时钟读数为

t_2 时这个光子回到原点，所以 $c=2\sqrt{(x^1)^2+(x^2)^2+(x^3)^2}/(t_2-t_1))$。现在我们在坐标系中的每个空间点上都放上一只全同的时钟，并且通过从原点发射一个球面电磁波（在所有方向上都有光子传播）来同步各点的时钟，即在 (x^1,x^2,x^3) 点接收到这个电磁波的瞬间把那里的时钟的时间调到 $\sqrt{(x^1)^2+(x^2)^2+(x^3)^2}/c$。于是，观察者现在可以在他的坐标系中给发生在当地的一个事件指定 3 个空间坐标以及一个时间坐标（这个时间坐标就是那里的时钟在事件发生的瞬间给出的读数）。我们也将假定我们所容许的观察者（无论他们是否有相对运动）是牛顿力学意义下的惯性观察者（即在我们所引进的坐标系中，一个不受力的粒子的轨迹或者是一个点或者一条以不变速度运动的直线）。一个相当明显的实验事实是，所有可容许的观察者都会承认同样的真空光速的数值（$c\approx 3.00\times 10^{10}\,\mathrm{cm}\cdot\mathrm{s}^{-1}$）①。我们将设想，所有可容许的观察者起初在某种距离单位上测量时间，这个距离就是用他们的时间坐标 t 乘以 c。最后，时间坐标定义为 $x^4=ct$。在这种单位下，所有速度都是无量纲的且真空光速等于 1。

在我们的事件世界的数学模型 $\mathcal{M}$ 中，可容许的观察者这种极为微妙和复杂的概念与可容许的基矢 $\{e^1,e^2,e^3,e^4\}$ 的简单概念是完全等同的。如果 $x\in\mathcal{M}$ 是一个事件且若写成 $x=x^a e_a$，那么 (x^1,x^2,x^3) 就是由相应的观察者确定的 x 空间坐标，而 x^4 则是时间坐标。如果 $\{\hat{e}^1,\hat{e}^2,\hat{e}^3,\hat{e}^4\}$ 是由方程[1]同 $\{e^1,e^2,e^3,e^4\}$ 联系在一起的另一组基矢/观察者，并且定义 $x=\hat{x}^a\hat{e}_a$，那么

$$\hat{x}^a=\Lambda^a_b x^b,\quad a=1,2,3,4 \tag{2}$$

因此，洛伦兹变换把两个可容许的观察者对于任何一个给定的事件的测量所分别得到的空间和时间坐标联系了起来。如果 $(\Lambda^a_b)\in\mathcal{R}$，那么这两个观察者的差别只在于他们各自空间坐标轴的取向不同。另一方面，对于任意一个实数 θ，可以定义 L 的一个元素：

$$L(\theta)=\begin{pmatrix}\cosh\theta & 0 & 0 & -\sinh\theta\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ -\sinh\theta & 0 & 0 & \cosh\theta\end{pmatrix} \tag{3}$$

而且如果两组可容许的基矢由这个洛伦兹变换联系起来，那么坐标变换[2]成为

$$\begin{aligned}\hat{x}^1&=(\cosh\theta)x^1-(\sinh\theta)x^4\\ \hat{x}^2&=x^2\\ \hat{x}^3&=x^3\\ \hat{x}^4&=-(\sinh\theta)x^1+(\cosh\theta)x^4\end{aligned} \tag{4}$$

令 $\beta=\tanh\theta$（因而 $-1<\beta<1$）并且假定 $\hat{x}^2=x^2$ 和 $\hat{x}^3=x^3$，则得到

$$\begin{aligned}\hat{x}^1&=\frac{1}{\sqrt{1-\beta^2}}x^1-\frac{\beta}{\sqrt{1-\beta^2}}x^4\\ \hat{x}^4&=-\frac{\beta}{\sqrt{1-\beta^2}}x^1+\frac{1}{\sqrt{1-\beta^2}}x^4\end{aligned} \tag{5}$$

① 这里需要强调的是，如果把这里的说法理解成是指双程平均真空光速就没有问题，但是如果本文作者在这里指的是单向真空光速则是错误的。因为至今为止，单向光速从来就没有被实验测量过，而且也不可能（除非找到光信号之外的对钟方法）用实验进行测量。真空光速在各个方向上都是 c 只是一种科学假定——译者注。

这个变换相应于空间坐标轴取向如图 2 所示的两个观察者,其中戴帽子的坐标系统沿共同的 x^1,$\hat{x}^1$ 轴以速度 $|\beta|$ 运动,如果 $\beta>0$ 向右运动,如果 $\beta<0$ 则向左运动。

我们要说,回到通常的时间单位的话,$\beta=v/c$,其中 $|v|$ 是两个坐标系之间的相对速度,而且方程[5]就成为狭义相对论中通常所说的"洛伦兹变换",即

$$\hat{x}^1=\frac{x^1-vt}{\sqrt{1-v^2/c^2}}$$
$$\hat{t}=\frac{t-(v/c^2)^1}{\sqrt{1-v^2/c^2}} \tag{6}$$

我们知道,要想了解狭义相对论的运动学效应,只要考虑所谓的特殊洛伦兹变换 $L(\theta)$ 就足够了。具体来说,我们可以证明(Naber 1992,定理 1.3.5),如果 $\Lambda\in L$ 是任意一个洛伦兹变换,那么就存在一个实数 θ 和两个转动 R_1,$R_2\in\mathcal{R}$,使得 $\Lambda=R_1L(\theta)R_2$。因为 R_1 和 R_2 不包含相对运动,所以全部的运动学都包含在 $L(\theta)$ 之中。

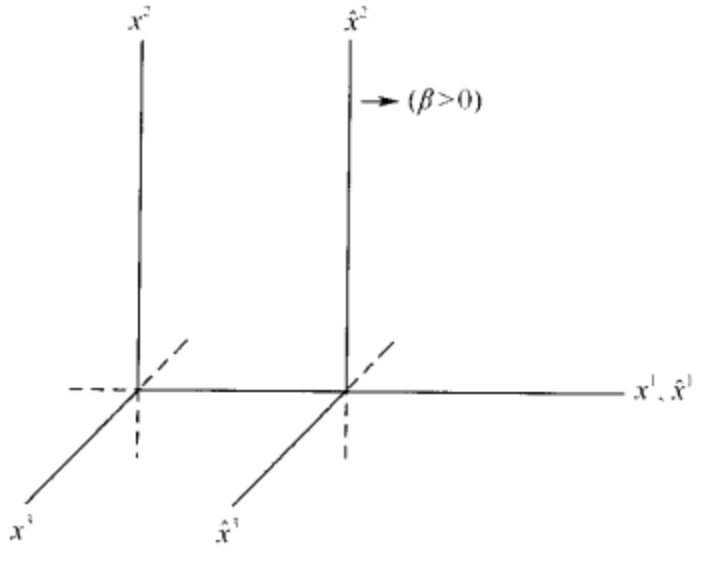

图 2 标准形式的观察者。

现在假定,x 和 x_0 是 $\mathcal{M}$ 中的两个不同事件,并考虑从 x_0 到 x 的平移矢量 $x-x_0$。如果 $\{e^1,e^2,e^3,e^4\}$ 是一个可容许的基矢,如果定义 $x=x^ae_a$ 和 $x=x_0^ae_a$,那么 $x-x_0=(x^a-x_0^a)e_a=\Delta x^ae_a$。如果 $x-x_0$ 是零矢量,那么

$$(\Delta x^1)^2+(\Delta x^2)^2+(\Delta x^3)^2=(\Delta x^4)^2$$

这就是说,两个事件的空间间隔等于光在这两个事件之间的时间间隙中传播的距离。这种情况对于其他任何可容许的基矢一样正确,因为洛伦兹变换是线性映射的矩阵,它们保持洛伦兹内积不变。因而,所有可容许的观察者都会有一致的结论,即 x_0 和 x 是"可以由光子联系起来"的。他们甚至还会一致看到两个事件中的哪一个是"发射"光子的,哪一个是"接受"光子的,因为可以证明(Naber 1992, 定理 1.3.3),如果一个非零矢量是类时矢量或零矢量,那么在每个可容许的基矢下它的 4 个坐标的符号都是一样的(因为 $\Lambda_4^4\geqslant1$)。所以,$x^4-x_0^4$ 要么对于所有可容许的观察者是正的(x_0 发生在 x 之前),要么对于所有可容许的观察者是负的(x_0 发生在 x 之后)。由于光子在可容许的坐标系中沿直线运动,所以我们将采用下面的术语。如果 $x_0,x\in\mathcal{M}$ 使得 $x-x_0$ 成为零矢量,那么在 $\mathcal{M}$ 中包含 x 和 x_0 的直线称为 $\mathcal{M}$ 中的光子的世界线,这条世界线被看作光粒子历史中经历的所有事件(包含 x 和 x_0 事件)的集合。

让我们现在另外假定 $x-x_0$ 是类时矢量。那么,在任意可容许的基矢下,

$$(\Delta x^1)^2+(\Delta x^2)^2+(\Delta x^3)^2<(\Delta x^4)^2$$

即两个事件 x_0 和 x 的空间间隔小于光在这两个事件之间的时间间隙中传播的距离。在这种情况下,我们可以证明(Naber 1992, 1.4 节),一定存在这样一个可容许的基矢 $\{\hat{e}^1,\hat{e}^2,\hat{e}^3,\hat{e}^4\}$,在这个基矢下 $\Delta\hat{x}^1=\Delta\hat{x}^2=\Delta\hat{x}^3=0$,即存在这样一个观察者,在他看来,这两个事件一先一后地发生在空间中的同一位置。设想这个位置被某个质点所占据(例如,放在这个位置上的观察者的时钟),我们发现,事件 x_0 和 x 都是这个质点所"经历"的,而

且$\sqrt{|g(x-x_0,x-x_0)|}$就是由这个质点携带的时钟所记录下的这两个事件之间的时间间隔。对于其他任意的可容许的观察者来说,这个质点看起来是"自由的"(即不受力),因为它会以不变的速度沿一条直线运动。这使我们有了下面的定义。如果$x_0,x\in\mathcal{M}$使得$x-x_0$是类时的,那么在$\mathcal{M}$中包含x_0和x的直线称为一个自由质点在$\mathcal{M}$中的世界线,而且$\sqrt{|g(x-x_0,x-x_0)|}$(这个量通常写成$\tau(x-x_0)$,或者简写成$\Delta\tau$)是x_0和x之间的固有时间间隔。我们可以把$\tau(x-x_0)$看成是$x-x_0$的一种"长度",是由一个经历了x_0和x这两个事件的自由粒子携带的时钟所测量的。然而,这是一种奇特类型的长度,因为它满足的不是通常的三角不等式,而是下面的"反转"形式。

反转三角不等式(Naber 1992, 定理 1.4.2) 设x_0,x和y是$\mathcal{M}$中那样的事件,使得$y-x$和$x-x_0$是具有同样时间取向的类时矢量。那么$y-x_0=(y-x)+(x-x_0)$就是类时的,而且

$$\tau(y-x_0)\geqslant\tau(y-x)+\tau(x-x_0) \qquad [7]$$

其中等号只有(当且仅当)$y-x$和$x-x_0$是线性无关时才成立。

不等式[7]导致很有意思的结果,稍后我们将对此介绍。

最后,考虑$x-x_0$是类空矢量的情况。这时,在任何容许的基矢下有

$$(\Delta x^1)^2+(\Delta x^2)^2+(\Delta x^3)^2>(\Delta x^4)^2$$

即两个事件x_0和x的空间间隔大于光在这两个事件之间的时间间隙中传播的距离。现在不会存在那样一个可容许的观察者,在他看来这两个事件能够发生在空间的同一个位置。也不可能存在那样一个自由粒子(即或是光子)能够经历这两个事件。然而,可以证明(Naber 1992, 1.5 节),给定任意一个实数 T(正、负或零),我们可以找到这样一个可容许的基矢$\{\hat{e}_1,\hat{e}_2,\hat{e}_3,\hat{e}_4\}$,在这个基矢下有$\Delta\hat{x}^4=T$。一些可容许的观察者判定这两个事件同时发生,另一些观察者则断言事件x_0发生在事件x之前,但是其他的观察者的判断相反。这种类型的两个事件的时间先后次序,即原因和结果,没有意义。对于能够断定这两个事件同时发生($\Delta\hat{x}^4=0$)的那些可容许的观察者而言,$\sqrt{g(x-x_0,x-x_0)}$这个量就是它们之间的距离,因而这个量称为x_0和x之间的固有空间距离(无论$x-x_0$是否类空)。

对于任意两个事件$x_0,x\in\mathcal{M}$,$g(x-x_0,x-x_0)$是在任意可容许的基矢下由$(\Delta x^1)^2+(\Delta x^2)^2+(\Delta x^3)^2-(\Delta x^4)^2$给出的,并被称为事件$x_0$和$x$之间的间隔。闵可夫斯基几何中的这种长度间隔非常类似于欧几里得几何中的(平方)长度。然而,依据事件x_0和x之间的物理关系,这两个事件之间的间隔可以是任意实数。当然,历史上对我们上面说的事件间隔曾有过各种物理解释,这种事件间隔的时空结构是以闵可夫斯基的名字命名的(Einstein et al. 1958)。

运动学效应

狭义相对论的所有熟知的运动学效应(速度相加公式、同时性的相对性、时间膨胀、长度收缩)全都很容易从上面的讨论来获得。鉴于前面已经说过的原因,我们将只限于讨论特殊洛伦兹变换。

设θ_1和θ_2是两个实数,考虑方程[3]定义的L的相应元素$L(\theta_1)$和$L(\theta_2)$。$\sinh\theta$和

$\cosh\theta$ 的求和公式意味着 $L(\theta_1)L(\theta_2)=L(\theta_1+\theta_2)$。定义 $\beta_i=\tanh\theta_i$，$i=1,2$，以及 $\beta_i=\tanh(\theta_i+\theta_2)$，那么对 $\tanh\theta$ 的求和给出

$$\beta=\frac{\beta_1+\beta_2}{1+\beta_1\beta_2} \qquad [8]$$

其物理解释很简单。设存在 3 个可容许的观察者，其空间坐标轴之间的关系如图 2 所示。如果第二个观察者相对于第一个的速度是 β_1，而第三个相对于第二个的速度是 β_2，那么第三个相对于第一个的速度就不是牛顿速度相加公式给出的 $\beta_1+\beta_2$，而是由式[8]给出的 β。这就是相对论的速度相加公式。

我们已经看到，如果 x_0 和 x 之间的间隔是类空的，那么这两个时间在某些可容许的观察者看来是同时发生的，而在其他观察者看来则不是。事实上，如果 $\Delta x^4=0$ 并且这些观察者由式[5]联系起来，那么 $\Delta\hat{x}^4=-(\beta/\sqrt{1-\beta^2})\Delta x^1=-\beta\Delta\hat{x}^1\neq 0$（除非 $\beta=0$，即没有相对运动），（$\Delta\hat{x}^1$ 不可能是零，因为会有 $\Delta\hat{x}^a$ 对于 $a=1,2,3,4$，即 $x=x_0$）。这种现象称为同时性的相对性，我们现在可以对这一现象进行简单的几何说明。

在平面中选取两条互相垂直的直线来代表 x^1 轴和 x^4 轴（这两条线的欧几里得垂直性没有物理意义，而且并非必要，但是可以使图像一目了然）。$\hat{x}^1$ 轴将由 $\hat{x}^4=0$ 的直线代表，按照式[5]，这将由 $x^4=\beta x^1$ 给出（在图 3 我们已经假定 $\beta>0$）。类似地，$\hat{x}^4$ 轴就是直线 $x^4=(1/\beta)x^1$。因为洛伦兹变换保持洛伦兹内积不变，双曲线 $(\Delta x^1)^2-(\Delta x^4)^2=k$ 与 $(\Delta\hat{x}^1)^2-(\Delta\hat{x}^4)^2=k$ 且我们相应地调整坐标轴的刻度使得（举例说）$(\Delta x^1)^2-(\Delta x^4)^2=1$（其中 $x^1>1$）与 x^1 轴在点 $(x^1,x^4)=(1,0)$ 相交。这需要在戴帽子的和不戴帽子的坐标轴有不同的刻度，但是可以证明（Naber 1992，1.3 节）在这样的刻度下，所有坐标值都可以做平行于对面的轴进行投影而得到（例如，一个时间的 x^4 坐标和 $\hat{x}^4$ 坐标可以分别做平行于 x^1 轴和 $\hat{x}^1$ 轴的投影而得到）。

因此，戴帽（或不戴帽）坐标的一条同时性直线平行于 $\hat{x}^1$ 轴（或 x^1 轴），所以一般情况下在一条同时性直线上的一对事件将不会在另一条同时性直线上（然而要注意，这些直线“实际上”都是三维超平面，所以我们所说的交点实际上是“相应的平面”，在其上的任何两个事件都会被这两个观察者看做是同时发生的）。

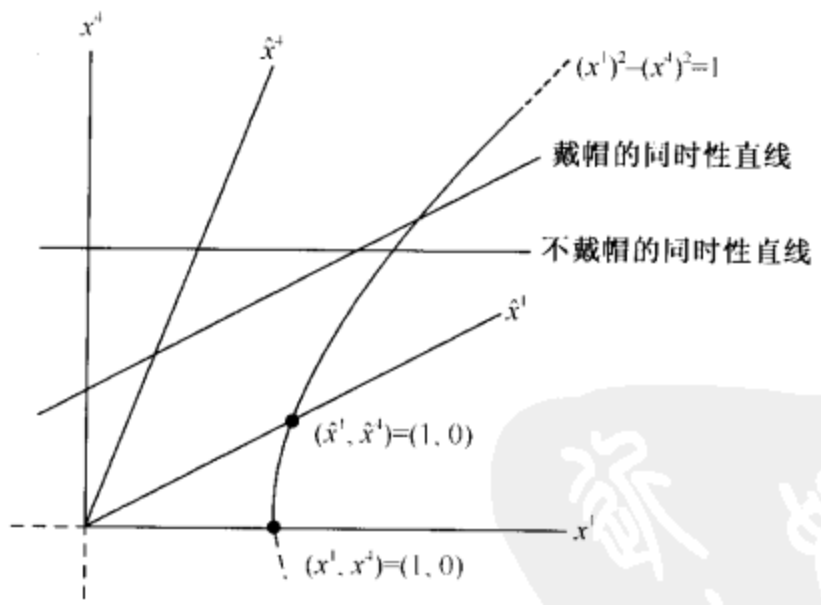

图 3　同时性的相对性。

无论如何，对应于任何两个事件，戴帽坐标的事件间隔 $\Delta\hat{x}^4$ 与不戴帽坐标的事件间隔 Δx^4 之间的关系由式[5]给出，

$$\Delta\hat{x}^4=-\frac{\beta}{\sqrt{1-\beta^2}}\Delta x^1+\frac{1}{\sqrt{1-\beta^2}}\Delta x^4$$

所以一般情况下这两个时间间隔不相等。例如，特别考虑静止在不戴帽的坐标系中的一个点的世界线上的两个事件，也就是静止在这个坐标系原点的一只始终的两个读数。这

种情况是 $\Delta x^1=0$，所以

$$\Delta\hat{x}^4=\frac{1}{\sqrt{1-\beta^2}}\Delta x^4>\Delta x^4$$

这种效应是完全对称的，因为，如果 $\Delta\hat{x}^1=0$，那么式[5]给出

$$\Delta x^4=\frac{1}{\sqrt{1-\beta^2}}\Delta\hat{x}^4>\Delta\hat{x}^4$$

每个观察者都认为其他的(运动)时钟走得慢。这种现象称为时间膨胀，这在图 4 的时空图中一目了然(例如，两个观察者都看到不戴帽坐标系原点上的时钟读数“0”，但是直线 $\Delta\hat{x}^4=1$ 与这个时钟的世界线即 x^4 轴在下面的一点 $(x^1,x^4)=(0,1)$ 相交)。

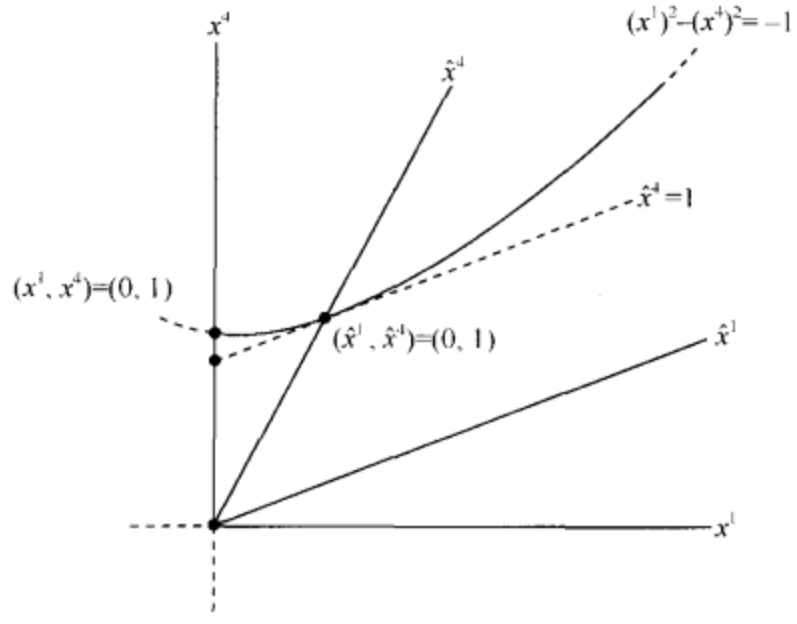

图 4　时间膨胀。

我们要强调的是，这种现象的物理意义是完全“真实的”。例如，在宇宙线里发现的某类粒子(介子)的寿命是如此之短以至于它们即使以光速运动，它们穿透地球大气层所需要的时间也要比它们的通常寿命大几十倍。如此，它们不可能到达地面，但是它们到达了。时间膨胀“使它们保持年轻”，即在我们看来它们的寿命要比通常的寿命长很多。

最后，因为不同的可容许的观察者一般来说对于时间是否同时发生看法不同，而且测量一个运动物体“长度”的惟一方法就是要(例如，用一把量尺)“同时”测量这个运动物体的两端；所以我们不应当奇怪，不同的可容许的观察者测量的长度(像同时性那样)和时间会不同。具体考虑一把沿戴帽坐标系 $\hat{x}^1$ 轴静止放置的测量尺子。在这个坐标系中它的“长度”是 $\Delta\hat{x}^1$。这把尺子的两个端点的世界线是平行于 $\hat{x}^4$ 轴的两条直线。如果不戴帽的观察者在这些世界线上同时观测两个事件，那么他们的坐标将满足 $\Delta x^4=0$ 且由式[5]有 $\Delta\hat{x}^1=(1/\sqrt{1-\beta^2})\Delta x^1$，那么

$$\Delta x^1=\sqrt{1-\beta^2}\,\Delta\hat{x}^1<\Delta\hat{x}^1$$

并且运动的量尺在其运动方向上缩短了 $\sqrt{1-\beta^2}$ 倍。就像时间膨胀那样，这种被称为长度收缩的现象式完全对称的、实在的，在时空图中是一目了然的(图 5)。

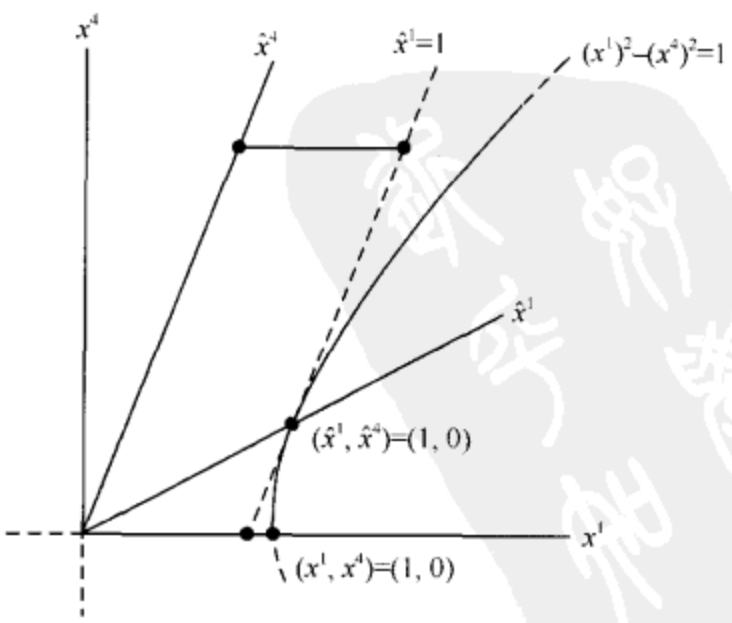

图 5　长度收缩。

相对性原理

我们已经看到，不同的可容许观察者对一些特别的事情可以有不同的结论(这些事情包括：两个事件是否同时、相对于各个观察者来说都不是同时发生的两个事件之间的时间间隔，以及量尺的长度等)。完全不用关心

的是在任何给定的情况下我们是否能够确定谁对。当然,两个事件要么同时发生要么不是,我们只需要分出哪些可容许观察者的观点是正确的?遗憾的是(或者侥幸的按照某种观点),不同的可容许观察者所给出的不同结论在物理上是完全不能允许的。

相对性原理(Einstein et al. 1958)*所有的可容许观察者对于物理定律的陈述都是等价的。*

我们必须清楚,这并不是一种数学陈述。那是一种对我们周围物理世界的精确的陈述,我们还要清楚如何从观察到的现象中提炼出来描写这种陈述;这些观测现象中的一些现象是复杂而难以琢磨的,而另一些现象则是平凡的(例如,在相对于地面以不变速度平稳飞行的飞机上的乘客不可能"感觉到"他相对于地球的运动)。相对性原理对于我们构造相对论性物理学定律是一种强有力的指导,但是更基本地是使我们避免把任何一个特别的可容许观察者对宇宙的看法当成是权威观点。特别是,它使我们避免认为下面一些问题具有客观的重要性:例如,"两颗超新星是同时爆发的吗?","介子存活了多长时间?,还有"蟹状星云和半人马星座 α 星之间有多远?" 这是极困难的问题,但是我们必须面对。

粒子和 4 动量

如果 $I\subseteq R$ 是一种间隔,那么映射 $\alpha: I\to\mathcal{M}$ 是 $\mathcal{M}$ 中的一条曲线。相对于任何可容许的基矢,对于每一个 $\xi\in I$,我们可以写下

$$\alpha(\xi) = x^a(\xi)e_a$$

假设 α 在如下意义上是平滑的:每个 $x^a(\xi)$,$a=1,2,3,4$,在 I 上是无限可微分的(C^∞),而且速度矢量

$$\alpha'(\xi) = \frac{\mathrm{d}x^a}{\mathrm{d}\xi}e_a$$

对于每个 $\xi\in I$ 都不会是零(我们采用通常的惯例,把每一点的切空间与这个矢量本身等同起来)。这种光滑性的定义显然与 M 中的可容许基矢的选取无关。如果对于每一点 $\xi\in I$

$$\alpha'(\xi)\cdot\alpha'(\xi) = \eta_{ab}\frac{\mathrm{d}x^a}{\mathrm{d}\xi}\frac{\mathrm{d}x^b}{\mathrm{d}\xi}$$

是正的、负的或者零,那么这条曲线 α 就分别被称为类空曲线、类时曲线或者零曲线。如果一条类时曲线 α 在每一点 $\xi\in I$ 上的 $\alpha'(\xi)$ 都指向未来,那么这条曲线就称为类时世界线,而且它的像点与某个质点(不必是自由质点)的历程中的全部事件的集合等同。如果 $I=[\xi_0,\xi_1]$,并且如果 $\alpha:[\xi_0,\xi_1]\to\mathcal{M}$ 是一条类时世界线,那么 α 的固有时间间隔被定义为

$$\begin{aligned}L(\alpha) &= \int_{\xi_0}^{\xi_1}\sqrt{|g(\alpha'(\xi),\alpha'(\xi))|}\,\mathrm{d}\xi\\ &= \int_{\xi_0}^{\xi_1}\sqrt{-\eta_{ab}\frac{\mathrm{d}x^a}{\mathrm{d}\xi}\frac{\mathrm{d}x^b}{\mathrm{d}\xi}}\,\mathrm{d}\xi\end{aligned}$$

而且被解释为 $\alpha(\xi_0)$ 和 $\alpha(\xi_1)$ 这两个事件的时间间隔,这个时间间隔是由那样一只时钟记录的,这只时钟是被具有世界线 α 的质点携带的。这种解释通过把其中的积分做黎曼求和近似而很容易引导出来,而且与我们关于固有时间间隔 $\Delta\tau=\sqrt{-\eta_{ab}\Delta x^a\Delta x^b}$ 的解释相

呼应。然而在数学和物理上都很精湛(Naber 1992, 1.4 节)。数学解释由下面的结果给出(这个结果同 Naber (1992)的定理 1.4.6 和 1.4.8 相结合)。

定理 设 x_0 和 x 是 $\mathcal{M}$ 中的两个事件,则 $x-x_0$ 是类时的并且指向未来,当且仅当在 M 中存在一条类时世界线 $\alpha:[\xi_0,\xi_1]\to\mathcal{M}$,其中有 $\alpha(\xi_0)=x_0$ 和 $\alpha(\xi_1)=x$,而且在这种情况下,

$$L(\alpha)\leqslant\tau(x-x_0) \qquad [9]$$

其中,等号只在 α 是一条类时直线的参数的情况下成立。

不等式[9]显示,如果两个质点都经历了 x_0 和 x,那么自由的那一个(也就是静止在某个可容许的坐标系中)会需要更长的时间等候第二个事件发生(运动的时钟走慢了)。多年以来,这种基本上明显的事实被命名为"孪生子佯谬"。

正如欧几里得中的一条曲线具有弧长参数那样,一条类时世界线具有如下定义的固有时参数。对于在$[\xi_0,\xi_1]$中的每一个 ξ,设

$$\tau=\tau(\xi)=\int_{\xi_0}^{\xi}\sqrt{|g(\alpha'(\zeta),\alpha'(\zeta))|}\,\mathrm{d}\zeta$$

(α 从 $\alpha(\xi_0)$到 $\alpha(\xi)$的固有时长度),那么 $\tau=\tau(\xi)$就有一个逆函数 $\xi=\xi(\alpha)$,所以 α 可以用 τ 来参数化。我们将稍微妄用我们的记号并写成

$$\alpha(\tau)=x^a(\tau)e_a$$

具有这种参数的速度矢量被定义为

$$U=U(\tau)=\frac{\mathrm{d}x^a}{\mathrm{d}\tau}e_a$$

这个速度矢量叫世界线的 4 速度,而且它是对 α 的单位切矢量,即对于每一个 τ

$$U(\tau)\cdot U(\tau)=-1 \qquad [10]$$

当然,一个可容许的观察者更可能用他自己的时间坐标 x^4 来对世界线进行参数化。那么

$$\alpha'(x^4)=\frac{\mathrm{d}x^1}{\mathrm{d}x^4}e_1+\frac{\mathrm{d}x^2}{\mathrm{d}x^4}e_2+\frac{\mathrm{d}x^3}{\mathrm{d}x^4}e_3+e_4$$

所以

$$|g(\alpha'(x^4),\alpha'(x^4))|=1-\|V\|^2$$

其中

$$\|V\|=\sqrt{(\frac{\mathrm{d}x^1}{\mathrm{d}x^4})^2+(\frac{\mathrm{d}x^2}{\mathrm{d}x^4})^2+(\frac{\mathrm{d}x^3}{\mathrm{d}x^4})^2}$$

是粒子速度矢量

$$V=V(x^4)=\frac{\mathrm{d}x^1}{\mathrm{d}x^4}e_1+\frac{\mathrm{d}x^2}{\mathrm{d}x^4}e_2+\frac{\mathrm{d}x^3}{\mathrm{d}x^4}e_3=V^ie_i$$

在给定的可容许的坐标系中的通常量值。那么我们发现

$$U=(1-\|V\|^2)^{-1/2}(V+e_4) \qquad [11]$$

我们将把 $\mathcal{M}$ 中的一个有质量的粒子用(α,m)这样一对量来代表,其中 α 是一条类时世界线,m 是这个粒子的固有质量或者叫静止质量(它是一个正的常数)。如果每个 $\mathrm{d}x^a/\mathrm{d}\xi$,$a=1,2,3,4$,是常数,那么$(\alpha,m)$就是一个具有固有质量 m 的自由有质粒子。(α,m)的 4 动量定义为 $P=mU$。所以

$$P\cdot P=-m^2 \qquad [12]$$

在任何可容许的基矢下,我们写出

$$P = P^a e_a = mU^a e_a = m\frac{\mathrm{d}x^a}{\mathrm{d}\tau}e_a$$
$$= m(1-\|V\|^2)^{-1/2}(V+e_4) \qquad [13]$$

在这些坐标中,P 的"空间"部分是

$$P = \frac{m}{\sqrt{1-\|V\|^2}}V$$

如果$\|V\| \ll 1$,那么这个量近似于 mV。如把 m 等同于牛顿力学中的惯性质量(这是由那样一个观察者测量的,这个观察者相对于这个粒子的速度很小),那么这就是这个粒子的经典动量。稍微更为明显的是,如果把 $1/\sqrt{1-\|V\|^2}$ 按照(广义)二项定理展开,那么得到

$$P^i = \frac{m}{\sqrt{1-\|V\|^2}}V^i = mV^i + \frac{1}{2}mV^i\|V\|^2 + \cdots \quad i=1,2,3 \qquad [14]$$

这个方程给出了经典动量的分量加上"相对论性修正"。为了保持在形式上与牛顿力学的相似,我们经常把 $m/\sqrt{1-\|V\|^2}$ 称为这个粒子的"相对论质量",但是我们将不用这个名词。P 的第 4 分量由下式给出:

$$P^4 = -P\cdot e_4 = \frac{m}{\sqrt{1-\|\boldsymbol{v}\|^2}} = m + \frac{1}{2}m\|\boldsymbol{v}\|^2 + \cdots \qquad [15]$$

相应于牛顿动能项$(1/2)m\|V\|^2$ 的出现表明,P^4 是给定的可容许观察者对这个粒子测量的相对论性总能量,并被记为 E:

$$E = -P\cdot e_4 \qquad [16]$$

现在,我们必须理解物理学中的"能量"概念是一个微妙的概念,而且把 $-P\cdot e_4$ 称为能量没有确保其任何物理内容。这个名字是否合适只能由实验决定。特别是,我们应当问,在式[15]中出现 m 这一项是否同 P^4 代表粒子"能量"的观点相一致。观察$\|V\|=0$ 的情况(即粒子相对于观察者是静止的),那么式[15]给出

$$E = m(=mc^2,\text{在标准单位下}) \qquad [17]$$

这就表明,粒子即使静止也有能量。如果这种能量真的是物理学意义上的"能量",那么它就能够被释放出来并得到应用。当然,事实上这是可能的,并且已经被令人信服地证明了。

下面我们会看到,不只是有质量的粒子有"动量"和"能量",而且光子也有因而也应当有 4 动量(例如,证据是光电效应,在这种效应中光子与逃离原子中电子轨道的电子之间的碰撞)。然而,不像有质粒子,光子的特性不是固有质量而是频率 ν(或者波长 $\lambda=1/\nu$),它与能量 ε 的关系是 $\varepsilon=h\nu$(h 是普朗克常数),而且与观察者有密切关联(多普勒效应)。而且没有类比于"固有质量"的"固有频率",因为不存在那类可容许的、光子在其中能够静止的观察者。为了尝试模仿这种特性,我们考虑一点 $x_0\in\mathcal{M}$,一条指向未来的零矢量 N 和一个间隔 $I\subseteq R$。由公式

$$\alpha(\xi) = x_0 + \xi N \qquad [18]$$

定义的一条曲线 $\alpha: I\to\mathcal{M}$ 是光子通过点 x_0 的参数化世界线。对于零世界线,NL 可以在任何可容许的基矢下写成

$$N = (-N\cdot e_4)(d+e_4) \qquad [19]$$

其中

$$d=[(N\cdot e_1)^2+(N\cdot e_2)^2+(N\cdot e_3)^2]^{-1/2}[(N\cdot e_1)e_1+(N\cdot e_2)e_2+(N\cdot e_3)e_3] \qquad [20]$$

是这条世界线在相应空间坐标系中的方向矢量。现在,通过类比式[16],我们把 $\mathcal{M}$ 中的光子定义成形式如式[18]的 $\mathcal{M}$ 中的一条曲线,把 N 取成是光子的 4 动量并且光子的能量 ε 在可容许的基矢 $\{e_1,e_2,e_3,e_4\}$ 被写成

$$\varepsilon=-N\cdot e_4 \qquad [21]$$

那么,由式[19],

$$N=\varepsilon(d+e_4) \qquad [22]$$

相应的频率 ν 和波长 λ 则被定义为 $\nu=\varepsilon/h$ 和 $\lambda=1/\nu$。在另一组可容许的基矢下,有 $N=\hat{\varepsilon}(\mathrm{d}\hat{r}+\hat{e}_4)$,其中 $\mathrm{d}\hat{r}$ 和 $\hat{\varepsilon}$ 是方程[20]和[21]中相应物理量的戴帽的量。可以看出(Naber 1992,1.8 节)

$$\frac{\hat{\varepsilon}}{\varepsilon}=\frac{\hat{\nu}}{\nu}\frac{1-\beta\cos\theta}{\sqrt{1-\beta^2}}=(1-\beta\cos\theta)+\frac{1}{2}\beta^2(1-\beta\cos\theta)+\cdots \qquad [23]$$

其中 β 是两个空间坐标系的相对速度,θ 是(在不戴帽坐标系中)光子的方向 d 与戴帽坐标系运动方向之间的夹角。方程[23]是相对论多普勒效应公式,其中展开级数中的第一项是经典多普勒效应公式。

作为本章节的总结,来考察我们上面的定义所描写的那种类型的粒子之间的几个简单的相互作用,为此只假设 4 动量在这些相互作用中守恒。为了方便,我们将使用自由粒子这个词来表示一个自由的有质粒子或者光子。如果 $\mathcal{A}$ 是自由粒子的一个有限集合,那么 $\mathcal{A}$ 中的每个元素都有惟一的一个 4 动量,这个动量或者是指向未来的类时矢量,或者是零矢量。任何这种集合中的矢量求和都是类时的并指向未来,除非所有的矢量全是互相平行的零矢量,在这样的情况下矢量的求和是指向未来的零矢量(Naber 1992,引理 1.4.3)。我们把这样的求和称为 $\mathcal{A}$ 的总的 4 动量。现在把下面一种定义公式化,这个定义要被用来模仿自由粒子的一个有限集合,这个集合在某个事件中同(或许是新的)另一个自由粒子的有限集合相碰撞,而这个新的集合是在碰撞中出现的(例如,一个电子和一个质子碰撞而产生一个中子和一个中微子)。$\mathcal{A}$ 中的一个接触性相互作用是一个三角形 $(\mathcal{A},x,\tilde{\mathcal{A}})$,其中 $\mathcal{A}$ 和 $\tilde{\mathcal{A}}$ 是自由粒子的两个有限的集合,它们都不包含具有线性相关的 4 动量的粒子对(它们或许在物理上是不可区分的)而且 $x\in\mathcal{M}$ 是这样的事件,使得

(1)x 是 $\mathcal{A}$ 中的所以粒子的终点(即对于 $\mathcal{A}$ 中的一个粒子的每条世界线 $\alpha:[\xi_0,\xi_1]\to\mathcal{M},\alpha(\xi_1)=x$);

(2)x 是 $\tilde{\mathcal{A}}$ 中的所以粒子的起点,而且

(3)$\mathcal{A}$ 的总的 4 动量等于 $\tilde{\mathcal{A}}$ 的总的 4 动量。

严格地说,(3)称为 4 动量守恒。如果 A 只包含单个自由粒子,那么 $(\mathcal{A},x,\tilde{\mathcal{A}})$ 被称为衰变(例如,一个中子衰变到一个质子、一个电子和一个中微子)。

例如,讨论一个相互作用 $(\mathcal{A},x,\tilde{\mathcal{A}})$,其中 $\tilde{\mathcal{A}}$ 包含单个光子。$\tilde{\mathcal{A}}$ 的总的 4 动量是零矢量,所以对于 $\mathcal{A}$ 来说也是如此。因为 $\mathcal{A}$ 中的各个粒子的 4 动量是类时的和零的且是未来指向的,所以只有它们全是平行的零矢量的时候,它们的和才可能是零矢量。因为 $\mathcal{A}$ 不能包含不同的光子有平行的 4 动量,它是必定由单个光子组成,根据(3),这个光子的 4 动

量与 $\tilde{A}$ 中光子的相同。在本质上,"在 x 处什么事情也没发生"。我们得出结论,没有我们所限定那种类型的非平凡的相互作用能够在一个单个光子上发生而且其他的事情也不会发生。把 A 和 $\tilde{A}$ 的角色颠倒后表明,如果 4 动量守恒,一个光子就不能衰变。

下面,我们考虑一个单有质粒子衰变到两个有质粒子,例如,一个原子到 α 发射的自发蜕变。因此,考虑一个有接触的相互作用$(A, x, \tilde{A})$,其中 A 包含一个具有固有质量 m_0 的单个自由有质粒子,而 $\tilde{A}$ 包含两个自由有质粒子(一个的固有质量是 m_1,另一个是 m_2)。设 P_0, P_1 和 P_2 分别是相应于固有质量为 m_0, m_1 和 m_2 的有质粒子的 4 动量。那么 $P_0 = P_1 + P_2$。按照"翻转三角不等式",由于 P_1 和 P_2 是线性无关的且是指向未来的以及方程[12],则有

$$m_0 > m_1 + m_2 \qquad [24]$$

初始粒子的额外质量 $m_0 - (m_1 + m_2)$按照式[17]被认为是把 m_0 分成两部分所要求的能量的一种度量。稍微不同的说法是,$\tilde{A}$ 中的两个粒子结合而形成 A 中的一个粒子时,"结合能"贡献给了后面粒子的质量。

在最后的例子中,颠倒 A 和 $\tilde{A}$ 的角色提供了非弹性碰撞(两个具有质量 m_1 和 m_2 的有质自由粒子相碰撞并结合成具有质量 m_0 的第三个有质自由粒子)中所含有的那种接触性相互作用的事例。当然不等式[24]保持有效,更详细一点的分析(Naber 1992, 1.8 节)给出 $m_0 - (m_1 + m_2)$的一个近似公式,这可以同在这个碰撞中的动能损失的牛顿公式做比较(在经典上,能量被看做是从结合粒子中获得热量的形式)。对含有一个电子和一个光子的 A 和 $\tilde{A}$ 的相互作用的分析得到(Naber 1992, 1.8 节)所谓康普顿效应的公式。这种类型的例子在 Synge 的著作(1972,第 6 章,§ 14)中有很详细的分析。

荷电粒子和电磁场

$\mathcal{M}$ 中的一个荷电粒子由(α, m, q)代表,其中(α, m)是一个有质粒子而 q 是一个被称为这个粒子的电荷的非零实数。我们对荷电粒子的两件事情感兴趣。荷电粒子的存在会产生电磁场,而且这些荷电粒子又受到其他电荷所产生的电磁场的作用。

荷电粒子是通过改变它们的 4 动量来表现它们对外部电磁场的"反应"。这种反应的定量性质,也就是运动方程,通常被看做是所谓的洛伦兹 4 力定律,这个力作为 4 速度的线性函数表达为粒子的 4 动量在世界线上的每个点相对于固有时的变化速率。所以,在世界线上的每一点有

$$\frac{\mathrm{d}P(\tau)}{\mathrm{d}\tau} = q\tilde{F}_{\alpha(\tau)}(U(\tau)) \qquad [25]$$

其中,$\tilde{F}_{\alpha(\tau)}: \mathcal{M} \to \mathcal{M}$ 是在每个可容许的坐标系中由经典电场 E 和磁场 H 决定的线性变换(这里假定 q 对周围电磁场的贡献忽略不计,即(α, m, q)是一个"检验电荷")。可以把式[25]更简单地写成

$$\tilde{\boldsymbol{F}}(\boldsymbol{U}) = \frac{m}{q}\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}\tau} \qquad [26]$$

用 $\boldsymbol{U}$ 点乘式[26]的两边得到

$$\tilde{\boldsymbol{F}}(\boldsymbol{U}) \cdot \boldsymbol{U} = \frac{m}{q}\frac{\mathrm{d}U}{\mathrm{d}\tau} \cdot U = \frac{m}{2q}\frac{\mathrm{d}}{\mathrm{d}\tau}(U \cdot U) = \frac{m}{2q}\frac{\mathrm{d}}{\mathrm{d}\tau}(-1) = 0$$

因为任何指向未来的类时单位矢量 $\boldsymbol{u}$ 是某个荷电粒子的 4 速度,我们则发现对于任何这样的矢量都有 $\tilde{\boldsymbol{F}}(\boldsymbol{u})\cdot\boldsymbol{u}=0$,那么线性意味着对于任何类时矢量都有 $\tilde{\boldsymbol{F}}(\boldsymbol{v})\cdot\boldsymbol{v}=0$。如果 $\boldsymbol{u}$ 和 $\boldsymbol{v}$ 都是指向未来的类时矢量,那么 $\boldsymbol{u}+\boldsymbol{v}$ 就是类时的,所以 $0=\tilde{\boldsymbol{F}}(\boldsymbol{u}+\boldsymbol{v})\cdot(\boldsymbol{u}+\boldsymbol{v})=\hat{\boldsymbol{F}}(\boldsymbol{u})\cdot\boldsymbol{v}+\boldsymbol{u}\cdot\hat{\boldsymbol{F}}(\boldsymbol{v})$并且 $\tilde{F}(u)\cdot v=-u\cdot\hat{\boldsymbol{F}}(v)$。然而,$\mathcal{M}$ 中具有未来指向的类时基矢,所以对于所有的 $x,y\in\mathcal{M}$ 有

$$\tilde{\boldsymbol{F}}(x)\cdot y=-x\cdot\tilde{\boldsymbol{F}}(y) \qquad [27]$$

因此,在每一点,线性变换 $\tilde{\boldsymbol{F}}$ 相对于洛伦兹内积必须是反对称的。因此我们可以模仿 $\mathcal{M}$ 上的一个电磁场,为此对这个反对称线性变换的每一点分派一个荷电粒子的 4 动量,这个粒子的世界线通过这个点,而由于电磁场的存在这个粒子要经历 4 动量的改变。但是另一种稍微不同的观点更方便。注意到一个反对称的线性变换 $\tilde{\boldsymbol{F}}:\mathcal{M}\to\mathcal{M}$ 和洛伦兹内积一起决定了下面给出的双线性形式 $\boldsymbol{F}:\mathcal{M}\times\mathcal{M}\to\mathrm{R}$,

$$\boldsymbol{F}(x,y)=\tilde{\boldsymbol{F}}(x)\cdot y$$

这也是反对称的($\boldsymbol{F}(y,x)=\tilde{\boldsymbol{F}}(y)\cdot x=-\boldsymbol{F}(x,y)$),而且反过来,一个反对称的双线性形式惟一决定了一个反对称线性变换。现在,在 $\mathcal{M}$ 的每一点指派一个反对称双线性形式就是 $\mathcal{M}$ 上的一个 2 形式,并且我们使用这样的"形式"语言来表达经典电磁理论(对这种语言的简明介绍可以参见 Spivak 的著作(1965,第 4 章)。

在自然界给予的确定限制下,2 形式能够合理地代表 $\mathcal{M}$ 上的电磁场("麦克斯韦方程")。为了进行公式化,引入如下的电磁场源的 1 形式 J:如果 x^1,x^2,x^3,x^4 是 $\mathcal{M}$ 上的任意可容许的坐标系,那么

$$J=J_1\mathrm{d}x^1+J_2\mathrm{d}x^2+J_3\mathrm{d}x^3-\rho\mathrm{d}x^4 \qquad [28]$$

其中,$\rho:\mathcal{M}\to\mathbf{R}$ 是电荷密度函数,$J=J_1e_1+J_2e_2+J_3e_3$ 是电流密度矢量场(它们被看做是通常的"光滑"函数,由相应的可容许的观察者逐点测量的"单位体积中的电荷"和"单位面积单位时间的电荷流量")。现在,给出如下的正规定义:由 $\mathcal{M}$ 上的源的 1 形式 $\mathcal{J}$ 所决定的 $\mathcal{M}$ 上的电磁场是一个 $\mathcal{M}$ 上的 2 形式 F,它满足麦克斯韦方程

$$\mathrm{d}F=0 \qquad [29]$$

和

$$^*\,\mathrm{d}^*F=\mathcal{J} \qquad [30]$$

下面依次给出几个评论。我们已经选择的单位是:光速和麦克斯韦方程中的各种其他常数(介电常数 ε_0 和磁导率 μ_0)都是 1,而且在式[30]中 4π 的因子已经被"归一化掉了"。方程[30]中的 $*$ 是由洛伦兹内积和 $\mathcal{M}$ 中的选定取向所确定的 Hodge 星算符。这是 $\mathcal{M}$ 上的 p 形式到$(4-p)$形式的一种自然的同构

$$^*:\Omega^p(\mathcal{M})\to\Omega^{4-p}(\mathcal{M}),\quad p=0,1,2,3,4$$

而且最简单定义如下:设 x^1,x^2,x^3,x^4 是 $\mathcal{M}$ 上的任意可容许的坐标系。如果 $1\in\Omega^0(\mathcal{M})$ 是 $\mathcal{M}$ 上的不变函数(0 形式),它的取值是 $1\in\mathbf{R}$,那么

$$^*1=\mathrm{d}x^1\wedge\mathrm{d}x^2\wedge\mathrm{d}x^3\wedge\mathrm{d}x^4$$

是 $\mathcal{M}$ 上的体积形式。如果 $1\leqslant i_1<\cdots<i_k\leqslant4$,则 $*(\mathrm{d}x^{i_1}\wedge\cdots\wedge\mathrm{d}x^{i_k})$惟一地被下面的公式决定

$$(\mathrm{d}x^{i_1} \wedge \cdots \wedge \mathrm{d}x^{i_k}) \wedge {}^*(\mathrm{d}x^{i_1} \wedge \cdots \wedge \mathrm{d}x^{i_k}) = -\mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3 \wedge \mathrm{d}x^4$$

因此,例如,

$${}^*\mathrm{d}x^2 = \mathrm{d}x^1 \wedge \mathrm{d}x^3 \wedge \mathrm{d}x^4,\ {}^*(\mathrm{d}x^1 \wedge \mathrm{d}x^2) = -\mathrm{d}x^3 \wedge \mathrm{d}x^4,\ {}^*(\mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3 \wedge \mathrm{d}x^4) = -1$$

等。于是,如果 μ 是 $\mathcal{M}$ 上的一个 p 形式,那么

$$^{**}\mu = (-1)^{p+1}\mu \qquad [31]$$

(对于更为完整的讨论,可参见 Choquet-Bruhat 等人的著作(1977, 第 5 章 A3))。特别是,式[30]等价于

$$\mathrm{d}^*F = {}^*J \qquad [32]$$

在没有电荷的区域,即 $J=0$,式[29]和[32]成为无源的麦克斯韦方程

$$\mathrm{d}F = 0 \qquad [33]$$

和

$$\mathrm{d}^*F = 0 \qquad [34]$$

这就是说,F 和 ${}^*F$ 都是闭合的 2 形式。

$\mathcal{M}$ 上的任何 2 形式 F 在任意的可容许坐标系中可以写成 $F=(1/2)F_{ab}\mathrm{d}x^a \wedge \mathrm{d}x^b$(重复指标的求和惯例!),其中$(F_{ab})$是 F 的反对称矩阵。为了同物理学中使用的记号进行联系,我们引入如下的定义

$$(F_{ab}) = \begin{pmatrix} 0 & B^3 & -B^2 & E^1 \\ -B^3 & 0 & B^1 & E^2 \\ B^2 & -B^1 & 0 & E^3 \\ -E^1 & -E^2 & -E^3 & 0 \end{pmatrix} \qquad [35]$$

因此,

$$F = E^1\mathrm{d}x^1 \wedge \mathrm{d}x^4 + E^2\mathrm{d}x^2 \wedge \mathrm{d}x^4 + E^3\mathrm{d}x^3 \wedge \mathrm{d}x^4 + B^3\mathrm{d}x^1 \wedge \mathrm{d}x^2 + B^2\mathrm{d}x^3 \wedge \mathrm{d}x^1 + B^1\mathrm{d}x^2 \wedge \mathrm{d}x^3 \qquad [36]$$

计算 ${}^*F, \mathrm{d}F, \mathrm{d}^*F$ 和 ${}^*\mathrm{d}^*F$ 并且写下 $E=E^1e_1+E^2e_2+E^3e_3$ 和 $B=B^1e_1+B^2e_2+B^3e_3$,我们发现 $\mathrm{d}F=0$ 等价于

$$\mathrm{div}B = 0 \qquad [37]$$

和

$$\mathrm{curl}\ E + \frac{\partial B}{\partial t} = 0 \qquad [38]$$

而 ${}^*\mathrm{d}^*F=J$ 等价于

$$\mathrm{div}\ E = \rho \qquad [39]$$

和

$$\mathrm{curl}\ B - \frac{\partial E}{\partial t} = J \qquad [40]$$

方程[37]~[40]是麦克斯韦方程的更加通俗的表达式。

在 $\mathcal{M}$ 上的另一个可容许的坐标系 $\hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{x}^4$(由式[2]的第一式相联系)下,2 形式 F 将被写成 $F=(1/2)\tilde{F}_{ab}\mathrm{d}\hat{x}^a \wedge \mathrm{d}\hat{x}^b$。代入 $\hat{x}^a=\Lambda^a_\alpha x^\alpha$ 和 $\hat{x}^b=\Lambda^b_\beta x^\beta$ 则给出 $F=(1/2)(\Lambda^a_\alpha\Lambda^b_\beta\tilde{F}_{ab})\mathrm{d}x^\alpha \wedge \mathrm{d}x^\beta$,所以有

$$F_{\alpha\beta} = \Lambda^a_\alpha\Lambda^b_\beta\tilde{F}_{ab}, \quad \alpha,\beta = 1,2,3,4 \qquad [41]$$

现在假定描写一个匀速运动电荷的电磁场。按照相对性原理,究竟是认为电荷相对于一个"固定的"可容许观察者运动还是认为这个观察者相对于一个"静止的"电荷运动,完全是无关紧要的。因此,我们写出固定在戴帽坐标系原点的一个电荷产生的电场("库仑定律")且由方程[41]变换到一个相对于这个戴帽坐标系运动的不戴帽坐标系。相对于 $\hat{x}^1$, $\hat{x}^2, \hat{x}^3, \hat{x}^4$, 对于在空间原点放置的点电荷 q 的通常反平方定律给出 $\hat{B}=0$ 和 $\hat{E}=(q/\hat{r}^3)\hat{r}$, 其中 $\hat{r}=\hat{x}^1\hat{e}_1+\hat{x}^2\hat{e}_2+\hat{x}^3\hat{e}_3$ 和 $\hat{r}=[(\hat{x}^1)^2+(\hat{x}^2)^2+(\hat{x}^3)^2]^{1/2}$(注意,$\hat{E}$ 只是在 $\mathcal{M}$一绑有$\{\hat{e}_4\}$上定义的)。因此,

$$(\hat{F}_{ab})=\frac{q}{\hat{r}^3}\begin{pmatrix}0 & 0 & 0 & \hat{x}^1\\ 0 & 0 & 0 & \hat{x}^2\\ 0 & 0 & 0 & \hat{x}^3\\ -\hat{x}^1 & -\hat{x}^2 & -\hat{x}^3 & 0\end{pmatrix} \qquad [42]$$

很容易在其范围内证实,$(\hat{F}_{ab})$满足无源麦克斯韦方程。把 Λ 取成相应于式[5]的特殊洛伦兹变换,并把式[41]用式[42]给出的$(\hat{F}_{ab})$写出来,得到

$$E^1=q\left(\frac{\hat{x}^1}{\hat{r}^3}\right)$$

$$E^2=\frac{q}{\sqrt{1-\beta^2}}\left(\frac{\hat{x}^2}{\hat{r}^3}\right)$$

$$E^3=\frac{q}{\sqrt{1-\beta^2}}\left(\frac{\hat{x}^3}{\hat{r}^3}\right)$$

$$B^1=0$$

$$B^2=\frac{-q\beta}{\sqrt{1-\beta^2}}\left(\frac{\hat{x}^3}{\hat{r}^3}\right)$$

$$B^3=\frac{q\beta}{\sqrt{1-\beta^2}}\left(\frac{\hat{x}^2}{\hat{r}^3}\right)$$

要使用不戴帽的观察者在电荷通过他的空间原点是的瞬间所做的测量来表达这些方程。在式[5]中代入 $x^4=0$ 后得到

$$\hat{x}^1=\frac{1}{\sqrt{1-\beta^2}}x^1, \hat{x}^2=x^2, \hat{x}^3=x^3$$

所以

$$\hat{r}^2=\frac{1}{1-\beta^2}(x^1)^2+(x^2)^2+(x^3)^2$$

为了方便写成 $\hat{r}_\beta^2$。在式[42]做了这些代替后得到

$$E=\frac{q}{\sqrt{1-\beta^2}}\left(\frac{1}{r_\beta{}^3}\right)(x^1e_1+x^2e_2+x^3e_3)$$

$$=\frac{q}{\sqrt{1-\beta^2}}\left(\frac{1}{r_\beta{}^3}\right)r \qquad [43]$$

和

$$B=\frac{q}{\sqrt{1-\beta^2}}\left(\frac{1}{r_\beta{}^3}\right)(0e_1-\beta x^3e_2+\beta x^2e_3)$$

$$= \frac{q}{\sqrt{1-\beta^2}}\left(\frac{1}{r_\beta^3}\right)((\beta e_1)\times r) \qquad [44]$$

这是一个以速度 βe_1 匀速运动的电荷在其通过坐标原点的瞬时所产生的电磁场。当 $\beta \ll 1$, $r_\beta \approx r$,那么式[43]是说,一个缓慢运动电荷的电场近似于库仑场。在 $\beta \ll 1$ 的情况,[44]退化为 Biot-Savart 定律。

我们来考虑另一个简单应用,即一个荷电粒子(α, m, q)对电磁场的反应,对于某个可容许观察者而言,电磁场是不变场且是纯磁场。为了简单,假设对于这个观察者来说,$E=0$ 和 $B=be_3$,其中 b 是一个非零的常数。相应的 2 形式 F 具有分量(从式[35]得到)

$$(F_{ab}) = \begin{pmatrix} 0 & b & 0 & 0 \\ -b & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

相应的线性变换 $\hat{F}$ 相对于这组基矢具有同样的矩阵,所以如果 $\alpha(\tau)=x^a(\tau)e_a$ 和 $U(\tau)=U^a(\tau)e_a$,那么洛伦兹 4 力定律[26]退化为线性微分方程体系

$$\frac{dU^1}{d\tau} = \frac{bq}{m}U^2, \quad \frac{dU^2}{d\tau} = -\frac{bq}{m}U^1$$

$$\frac{dU^3}{d\tau} = 0, \quad \frac{dU^4}{d\tau} = 0$$

这个方程体系容易被求解且容易积分而给出

$$\alpha(\tau) = x_0 + a\sin\left(\frac{bq\tau}{m}+\phi\right)e_1 + a\cos\left(\frac{bq\tau}{m}+\phi\right)$$

$$+ c\tau e_3 + \left(1+\frac{a^2b^2q^2}{m^2}+c^2\right)\tau e_4 \qquad [45]$$

其中,$x_0 = x_0^a e_a \in \mathcal{M}$ 是常数,a,ϕ 和 c 是实的常数且 $a>0$(我们已经使用 $U\cdot U=-1$ 消去了另一个任意实的常数)。注意,在 α 上的每一点,$(x^1-x_0^1)^2+(x^2-x_0^2)^2=a^2$。因此,如果 $c\neq 0$,那么在这个坐标系中的空间轨迹是一条沿 e_3 方向(即磁力线方向)的螺旋线。如果 $c=0$,那么这条轨迹就是一个在 x^1-x^2 平面中的圆。这种情况具有某种实际意义,因为可以在气泡室中引入不变的磁场以使我们关注的那种粒子沿一个圆轨道运动。现在我们显示如何测量这样一种粒子的荷-质比。在方程[45]中取 $c=0$ 并且计算 $U(\tau)$,利用式[11]对粒子的坐标速度矢量求解后得到

$$\boldsymbol{v} = \frac{abq/m}{\sqrt{1-\|\boldsymbol{v}\|^2}}\left[\cos\left(\frac{bq\tau}{m}+\phi\right)e_1 + \sin\left(\frac{bq\tau}{m}+\phi\right)e_2\right]$$

由此计算

$$\|\boldsymbol{v}\|^2 = \left(1+\frac{m^2}{a^2b^2q^2}\right)^{-1}$$

(注意,这是个常数)。对 q/m(为了方便,假定 $q>0$)求解最后一个方程,得到

$$\frac{q}{m} = \frac{1}{a|b|}\frac{\|\boldsymbol{v}\|}{\sqrt{1-\|\boldsymbol{v}\|^2}}$$

因为 a,b 和 $\|\boldsymbol{v}\|$ 都是可测量的,所以能得到所要求的荷-质比。

为了得出结论,我们要简单讨论存在性并利用电磁场的“势”。假设 F 是定义在 $\mathcal{M}$

中的某个连通的开区域 X 上的电磁场。那么 F 就是 X 上的 2 形式，由式[29]知道它是闭合的。仍然假设，X 的第二种 *de Rham* 上同调 $H^2(X;\mathbf{R})$ 是平凡的（因为 $\mathcal{M}$ 在拓扑上是 $\mathbf{R}^4$，例如，当 X 是 $\mathcal{M}$ 的全体、或者是 $\mathcal{M}$ 中的一个开球、或者更一般地是 $\mathcal{M}$ 中的一个开的“星形式”的区域，都属于这种情况）。由定义，X 上的每个闭合的 2 形式都是恰当的，所以特别存在 X 上的一个 1 形式 A 满足

$$F = \mathrm{d}A \qquad [46]$$

特别是，对于任意 F 在 X 中的任意点的一个邻域总是局域地存在这样一个 1 形式 A。然而这样的 A 并不是被惟一确定的，因为如果 A 满足式[46]，那么 $A+\mathrm{d}f$ 也满足式[46]，其中（0 形式）f 是定义在 X 上的任意光滑的取实数值的函数（$\mathrm{d}^2=0$ 意味着 $\mathrm{d}(A+\mathrm{d}f)=\mathrm{d}A+\mathrm{d}^2f=\mathrm{d}A=F$）。任何满足式[46]的 1 形式 A 称为 F 的（规范）势。对于某个 f，平移 $A\to A+\mathrm{d}f$ 称为规范势的规范变换，并且这种不改变式[46]的平移的自由度称为规范自由度。

可以看出，给定 F，对于依 0 形式 ${}^*\mathrm{d}{}^*A$ 的任意细节而定的 A，总能够局域求解 $\mathrm{d}A=F$。更严格地说，如果 F 满足 $\mathrm{d}F=0$ 且 g 是任意的 0 形式，那么局域上，在任意点的邻域，存在一个 1 形式 A 满足

$$\mathrm{d}A = F \quad \text{和} \quad {}^*\mathrm{d}*A = g \qquad [47]$$

（在 Parrott 著作（1987，附录二）中证明了更一般的结果，而且在这同一著作中的 2.9 节还有一个更一般的情况）。方程[47]中的第二个条件可以如下描绘。假设给出有关电荷和电流的某种（物理）构成（即源的 1 形式 J）且想要求出相应的电磁场 F。我们必须求解麦克斯韦方程 $\mathrm{d}F=0$ 和 ${}^*\mathrm{d}{}^*F=J$（依边界条件是否合适而定）。至少在局域上可以寻求替代相应的规范势 A（所以 $F=\mathrm{d}A$），那么麦克斯韦方程组的第一个方程自动被满足（$\mathrm{d}F=\mathrm{d}(\mathrm{d}A)=0$）而且只需要求解方程 ${}^*\mathrm{d}{}^*(\mathrm{d}A)=J$。为了简化记号，我们暂时写成 $\delta={}^*\mathrm{d}*$ 且在考虑“形式”上的算子 $\Delta=\mathrm{d}\circ\delta+\delta\circ\mathrm{d}$（有各种不同的名称：Laplace-Beltrami 算子、Laplace-de Rham 算子，或者叫做闵可夫斯基时空上的 Hodge Laplacian）。则

$$\Delta A = \mathrm{d}(\delta A)+\delta(\mathrm{d}A) = \mathrm{d}({}^*\mathrm{d}{}^*A)+{}^*\mathrm{d}{}^*(\mathrm{d}A) \qquad [48]$$

按照上面给出的结果，利用 ${}^*\mathrm{d}{}^*A=0$ 的条件简化前面的讨论，于是

$$\delta A = 0 \qquad [49]$$

（这就是通常说的洛伦兹规范）。在这种规范下，式[48]成为 $\Delta A={}^*\mathrm{d}{}^*(\mathrm{d}A)$ 且要满足第二个麦克斯韦方程，必须求解

$$\Delta A = J \qquad [50]$$

因此，我们看到（局域）求解给定源 J 的麦克斯韦方程简化为对于规范势 A 来求解方程[49]和[50]。为了了解问题的求解是如何简化的，我们注意到，在可容许坐标系中的计算显示，算子 Δ 简化为在实数取值函数上定义的达朗贝尔算子 $\Box$，

$$\Box = \frac{\partial^2}{\partial(x^1)^2}+\frac{\partial^2}{\partial(x^2)^2}+\frac{\partial^2}{\partial(x^3)^2}+\frac{\partial^2}{\partial(x^4)^2}$$

因此，方程[50]退耦为 4 个标量方程：

$$\Box A_a = J_a, \quad a=1,2,3,4 \qquad [51]$$

进一步的阅读材料

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导论:量子力学

历史背景

这一节我们将简要回顾现代量子力学理论和形式的基本经验事实和最初的理论尝试。在下面的章节里,我们将给出量子力学的数学和计算结构,以及量子力学成功解决了的物理问题,并描述量子力学所导致的严重的概念自洽性问题(它们至今尚未得到解决)。

从 19 世纪 50 年代开始就已经发现。在光的吸收和发射现象中存在离散化的经验规则 Fraunhofer 注意到,太阳光的吸收谱线中的暗线和所有元素的发射谱线中的明线是重合的。G Kirchhoff 和 R Bunsen 得到结论:光的发射和吸收的相对强度意味着发射和吸收的能量比例是不依赖于所考虑的原子的。这是 Planck 分析的出发点。

另一方面,到 18 世纪末期,原子的空间结构得到了研究;其中最成功的是 Rutherford 模型:原子包含一个带正电荷 Z 的原子核和 Z 个与原子核有库仑吸引相互作用的电子。这个模型所描述的原子大小与牛顿定律和经典电动力学完全背离;实际上,根据这些定律,原子将是不稳定的,而且肯定不会出现离散的能谱。我们可以得出结论:经典的物理定律对于描述由原子内部结构支配的光的发射和吸收现象是不适当的。

旧量子理论一般认为是诞生在 M Planck 讨论黑体辐射的 1900 年。

Planck 提出假设:物质发射和吸收光只能通过能量正比于其频率的"共振子"的过程进行。将统计力学中的 Gibbs 规则应用于共振子气体,这个假设可以重现黑体辐射实验发现的定律(Planck 定律)。爱因斯坦根据这一规律将光(从 Maxwell 时代开始就被波动的语言成功地描述)赋予离散的、类似于粒子的性质。9 年以后爱因斯坦理论进一步证实了对 Planck 的假说支持:他证明 Planck 假说可以正确地描述黑体辐射的能量涨落,并且澄清了比热容的特性。不久以后,爱因斯坦(1924,1925)证明,假定的光粒子满足零质量粒子的相对论关系(即能量和动量的关系)。

Compton 效应实验和爱因斯坦对光电效应的描述(Einstein 1905)进一步的支持光的波粒二象性。需要强调的是,虽然 Planck 将光考虑为与物质相互作用而具有能量 $h\nu$($h=6.6\times10^{-27}\,\mathrm{erg}\cdot\mathrm{s}$),但爱因斯坦进一步赋予光量子粒子的(定域化)性质,这标志着对经典电磁学定律的完全背离。

"可以想像,在纯粹的光学现象上保留其有效性并建立在空间连续函数基础上的光的波动理论,在应用到有光的产生和转化的现象时,将导致与实验结果的矛盾;实际上,这些现象可以用这样的假设来更好地描述:光是不连续地分布在空间的,由有限数量的量子描述,这些量子能够运动但不可分割,且必须被整个的吸收或者发射。"

注意,对于 $8\times10^{2}\,\mathrm{nm}$ 的波长,一个 30W 的灯每秒大约发射 10^{20} 个光子;对于宏观物体来说,我们并未感知到光的离散性。

Planck 的假说和能量守恒意味着,在光的发射和吸收中各种元素的原子失去或者得到的能量只能取离散的值。所以,作为辐射的产生者或吸收者的原子能够被这样一个理

论更好地描述:每个原子具有一组离散的(可能为无穷多个)具有确定能量的状态。

物质的旧量子理论就是要准确地说明这个问题。它的主要提出者是 N Bohr(Bohr 1913,1918)。这个新的理论完全是唯象的(就像 Planck 理论那样),而且建立在原子的 Rutherford 模型和如下 3 个假定的基础上(Bohr 1924):

(i) 原子的态是由牛顿定律给出的稳定的周期运动轨道,其能量 E_n, $n\in Z^+$,由公式 $E_n=h\nu_n f(n)$给出,其中 h 是 Planck 常数,ν_n 是电子在该轨道上运动的频率,对于每一个原子,至少当 Z[①] 较小时,$f(n)$是一个 Z 的近似线性函数。

(ii) 在原子发射或者吸收能量的时候,原子就跃迁到另一个不同的状态。发射或者吸收的辐射的频率正好是 $\nu_{n,m}=h^{-1}|E_n-E_m|$。

(iii) 当 n 和 m 的数值很大且$(n-m)/(n+m)$的数值很小时,新理论的预言应该和物质与辐射相互作用的经典理论相一致。

后来,A Sommerfeld 给出了第一个假定的一种不同的版本:要求所允许的电子轨道的经典作用量是 Planck 常数的整数倍。

当应用到简单系统($Z<5$ 的原子)时,旧量子理论取得成功。但是很快变得明确的是,一种新的、根本上不同的观点和一个崭新的出发点是需要的;新的理论必须包含很少的自由参数,而假设(iii)的角色就是用来固定这些参数的数值。

历史上有两种(成功的)尝试来构造一个自圆其说的理论;两种理论都需要有更加明确定义的数学形式。第一种尝试是由 W Heisenberg 发起的,而进一步的重要的概念和数学支持则来自于 M Born, P Jordan, W Pauli, P Dirac 和数学方面也有贡献的 J von Neumann 与 A Weyl。这种理论主张只考虑可观测量之间的关系,这些关系由只依赖于系统的初态和末态的元素描述;每一个状态都具有一个能量。由于能量守恒,这些能量之间的差异应该(以一个普适常数)正比于吸收或者发射的频率。这足够定义单原子态的能量(只差一个常数)。这个理论也必须考虑在外电磁场影响下发生跃迁的几率。

我们会在后面给出这个理论的一些细节,这将帮助我们掌握这种处理方法的基本原理。

另外一种尝试由 L de Broglie 在 HW Bragg 和 M Brillouin 早期评论的影响下提出。与强调光的离散性质相反,利用经典力学中的 Hamilton-Jacobi 公式,他着重阐述了粒子可能的波动性质。这种尝试很快得到了 Davisson 和 Germer(1927)的离子束在晶体上的散射实验的支持。实验说明,虽然电子被记录时显现为"点状粒子",它们的分布却遵循(色散)波衍射的强度定律。而且,在实验误差范围内,电子动量和频率的关系与爱因斯坦得到的关于光子的结果是一样的。

de Broglie 的理论很快被 E Schrödinger 提出的几乎确定的理论形式代替。在这种处理方法里,人们很自然的被引导到建立和求解偏微分方程的路子上来,而理论的发展则需要来自函数理论的规律性的结果。

Schrödinger 很快意识到在 Heisenberg 的方法中发现的关系能够容易地(我们将稍后讨论技术细节)在他所倡导的理论形式中得到,并且他真的给出了两种理论形式等价的证明。这个证明后来被 J von Neumann 和 G Mackey 从数学的观点改进了。

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① 这里 Z 是原子携带的总电子数——译者注。

事实上,Schrödinger 的处理方法已经被证明在非相对论领域内求解物理问题更加有用,因为它能利用函数和偏微分方程理论的发展和实际应用。Heisenberg 的"代数"处理方法因而在解决(非相对论)量子力学的具体问题上成了次要的角色。

如果考虑粒子数随时间变化的过程,我们不得不引入可以容纳具有任意多粒子数状态的 Hilbert 空间,其情形正如相对论量子场论和量子统计力学;由于处理具有无穷多变量函数空间的困难,沿用 Schrödinger 的路线则是更为困难。建立在矩阵代数基础上的 Heisenberg 方法,具有向合适的算子代数的非常自然的推广;而建立在用(波)函数描写状态基础上的 Schrödinger 处理方法,由于人们必须引入函数空间上的泛函而遇到更多的困难,对于动力学的描述也不再具有简单的形式。

从这种观点出发,Heisenberg 方法的推广已经对理论结构的理解产生了很多的进步。当然,其中一些相关的结果已经用 Schrödinger 表象得到。我们将不对这一点做进一步的详细阐述。

我们将用一段在 Heisenberg 和 Schrödinger 框架内量子力学结构是如何出现的简短描述来结束这个介绍性的小节;这将提供一个我们将在下面一节介绍量子力学公理的动机。如果需要更加全面的分析,可以参考 Jammer(1979)的讨论。

由 de Broglie(1923)假定的粒子波动性质的特殊形式依赖于波传播的几何光学关系,以及通过求解 Hamilton-Jacobi 方程和引入群速度概念得到的一种"波前传播"的 Hamilton 力学公式。

考虑与电磁波的相似性,我们很自然地把一个动量为 p、质量为 m 的非相对论自由粒子与如下的平面波

$$\phi_p(x,t) = \mathrm{e}^{i(px-Et)/\hbar}, \hbar = \frac{\hbar}{2\pi}, E = \frac{p^2}{2m}$$

联系起来。考虑与电磁波在折射率为 $n(x,\omega)$(在波长尺度上缓慢变化)的介质中传播的相似性,Schrödinger 得到了量子粒子在势为 $V(x)$的保守力场中的方程。确实,在这种情况下,"波动"遵循几何光学的定律,因而具有了"类似粒子"的行为。如果我们用$\hat{u}(x,\omega)$表示一个电场普通分量的(对于时间的)傅里叶变换,并且假设场本质上是单色的(以至于 ω 的函数$\hat{u}(x,\omega)$主要分布在 ω_0 附近的一个非常小的邻域内),人们发现$\hat{u}(x,\omega)$是下面方程的一个近似解:

$$-\Delta\hat{u}(x,\omega) = \frac{\omega_0^2}{c^2}n^2(x,\omega)\,\hat{u}(x,\omega) \qquad [1]$$

记$\hat{u}(x,\omega) = A(x,\omega)\,\mathrm{e}^{i(\omega/c)W(x,\omega)}$,则相位 $W(x,\omega)$在高频极限下满足程函方程 $|\nabla W(x,\omega)|^2 = n^2(x,\omega)$。我们可以对其解定义一个相速度 v_f,而且可以证明 $v_f = c/|\nabla W(x,\omega)|$。

另一方面,经典力学也能够用 Hamilton-Jacobi 方程 $H(x,\nabla W) = E$ 解$W(x,\omega)$的水平曲面的传播来描写,其中 $H(x,p) = p^2/2m + V(x)$。记住,高频率(几何光学的区域)对应的是小距离。这个相似性导致 Schrödinger(1926)假定与粒子联系在一起的波满足的动力学由下面的(Schrödinger)方程给出:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta_x\psi(x,t) + V(x)\psi(x,t) \qquad [2]$$

这个波用来描述粒子及其运动,但是,由于值是复数的,它不能表示任何可观测的性质。方程[3]的解的一个数学性质是:量 $\int|\psi(x,t)|^2\mathrm{d}^3x$ 随着时间是保持不变的。进一步地,如果人们令

$$\rho(x,t)=|\psi(x,t)|^2,$$

$$j(x,t)=-i\frac{\hbar}{2m}[\bar{\psi}(x,t)\nabla\psi(x,t)-\psi(x,t)\nabla\bar{\psi}(x,t)] \qquad [3]$$

则容易检验定域守恒定律

$$\frac{\partial\rho}{\partial t}+\mathrm{div}j(x,t)=0 \qquad [4]$$

这些数学性质导致了由 Max Born 给出的统计诠释:在实验中对粒子的位置进行测量,则 $|\psi(x,t)|^2$ 在空间区域 Ω 上的积分给出在 t 时刻该粒子位于区域 Ω 内的几率。此外,带电粒子的定域电流由 $j(x,t)$ 给出。

现在我们简要地回顾 Heisenberg 的处理方法。处于这种方法核心地位的是:发射和吸收强度的经验公式(色散关系),Sommerfeld 的作用量量子条件,以及"对离散变量之导数的类似物对应于有限差商"这一含糊不清的表述。最重要的是,对原子物理的正确描述是通过与两个状态联系在一起的量,即(无穷维)矩阵,和在原子能级 k 和 $j(k\neq j)$ 之间的跃迁中(发射或者吸收的)辐射的频率(或者波数更合适)$\omega_{k,j}$ 满足 Ritz 组合规则 $\omega_{m,j}+\omega_{j,k}=\omega_{m,k}$ 这一经验事实来达到的。很容易看到任何满足这个关系的双指标的序列必须具有形式 $\omega_{m,k}=E_m-E_k$,其中 E_j 是合适的常数。

Kramers 经验性地检验了在频率为 ν 的单色外场中原子的电偶极矩正比于场强,比例系数(极化)为

$$P-\frac{e^2}{4\pi m}\sum_i\left[\frac{f_i}{\nu_i^2-\nu^2}-\frac{F_i}{\nu_i^2-\nu^2}\right] \qquad [5]$$

式中,e, m 是电子的电荷和质量,f_i, F_i 是频率为 ν 的发射或吸收几率。

用经典力学对极化现象的详细分析是 Max Born(1924)给出的,他宣称工作的目的是:给出的结果在某种程度上可能为构建新的力学提供线索。他假设原子可以被看成是频率为 ν_i 的、线性地与频率为 μ 的电场耦合的谐振子的集合,并使用了作用量-角变量 $\{J_i,\theta_i\}$。

在偶极近似下,人们得到如下的关于极化 P(能量对于电场的线性响应)的结果:

$$P=-\sum_{(\nu\cdot m)>0}2(m\cdot\nabla_J)\frac{|\boldsymbol{A}(J)|^2(\nu\cdot m)}{(m\cdot\nu)^2-\mu} \qquad [6]$$

式中,$\nu_k=\partial H/\partial J_k$,$H$ 是相互作用哈密顿量,$\boldsymbol{A}(J)$ 为一个合适的矩阵。以对应原理作为指导,为了得到新的动力学,人们必须将这个结果与 Kramers 色散关系比较。为了更容易地比较,我们将 Kramers 色散关系写为如下形式:

$$P=\frac{e^2}{4\pi m}\sum_{n,m}\frac{f_{m,n}}{\nu_{n,m}^2-\mu^2}-\frac{f_{n,m}}{\nu_{n,m}^2-\mu^2}\quad E_m>E_n \qquad [7]$$

Bohr 的规则意味着 $\nu(n+\tau)=(E(n+\tau)-E(n))/\hbar$。

Born 和 Heisenberg 注意到,对于足够大的 n 和足够小的 k,人们可以将式[6]中的微分算子近似为相应的差分算子,导致的误差是 k/n 量级的。因此,式[6]可以被代换为

$$P=-\hbar^{-1}\sum_{m_k>0}\left[\frac{|\boldsymbol{A}_{n+m,n}|^2}{\nu(n+m)^2-\mu^2}-\frac{|\boldsymbol{A}_{n-m,n}|^2}{\nu(n-m)^2-\mu^2}\right] \quad [8]$$

Born 和 Heisenberg 得到的结论是,取代经典理论中动量地位的矩阵 $\boldsymbol{A}$ 必须是 $|\boldsymbol{A}_{n+m,n}|^2=e^2\hbar m^{-1}f(n+m,n)$这样的形式。同样的道理,考虑在静电场中的极化,可能找到代替经典 Hamilton 理论中坐标 x 的矩阵的表达式。

一般而言,新的处理方法(矩阵力学)将矩阵和一些相关的经典可观测变量(例如,位置和动量的函数)由时间相关性联系起来,这可以由 Kramers 的经验色散关系、对应原理、Bohr 规则、Sommerfeld 作用量原理和原子与外电磁场作用的一级(和二级)微扰论推导出来。很快 Born 和 Jordan(1925)弄清楚了这种动力学具有 $i\hbar\dot{A}=A\boldsymbol{H}-\boldsymbol{H}A$ 这样的形式,其中矩阵 $\boldsymbol{H}$ 对于氢原子情形是对经典的哈密顿量中的坐标 x 和 p 作某种规定而得到的。也可以看出,对应于位置和动量的矩阵 $\hat{x}_k$ 和 $\hat{p}_k$,似乎有关系 $[\hat{x}_k,\hat{p}_k]=i\boldsymbol{I}$。一年以后 P Dirac(1926)指出这种关系与哈密顿动力学中泊松括号有相同的结构,发展出"量子代数"和"量子微分",而且证明了 $N\times N$ 矩阵的代数 $\mathcal{B}_N$ 的任意 * 导数 δ(保共轭的导数)是内(导数),而对于 Hermit 矩阵 $\boldsymbol{h}$,由 $\delta(a)=i[a,\boldsymbol{h}]$给出。很久以后这个定理被推广(伴随一些假设)到可分 Hilbert 空间全体有界算子的代数上。由于这种导数是单参数自同构连续群的生成元,也就是动力学的生成元,这个结果进一步加强了 Born 和 Heisenberg 的想法。

遵循库仑系统 $SO(4)$ 对称性辛力学的推导思路,由 Born, Jordan 和 Heisenberg (1926)引入的代数结构被 Pauli(1927)用来给出了一种对氢原子能谱的纯粹的群理论推导。这个非凡的成功给予量子力学的 Heisenberg 形式以很强的支持,很快被公认为研究原子世界的有效工具。

代数形式在 Pauli(1928)对"自旋"(为了解释一些发射谱线的超精细分裂,它被 Goudsmidt 和 Uhlenbeck 经验性地假定为电子的一种性质)做出描述的时候也得到了应用。自旋被描写为一种不涉及空间坐标的"内部"自由度,而且在空间转动群的作用下仍然与系统的性质联系在一起。矩阵描述在 Pauli 给出不相容原理的形式(以及和 Fermi-Dirac 统计的联系)中也扮演了主要的角色,并通过正确地重现原子的分类给予 Heisenberg 的理论以进一步的声誉。

这些特征也许解释了为什么下一节中给出的量子力学公理的标准形式显示出 Heisenberg 处理方法的影响。另一方面,与实验的比较通常出现在 Schrödinger 方法的框架内。由于 Schrödinger 方程的解的性质造成的困惑,致使人们只关注理论形式的实际应用,而把诠释的困难放在一边。这样的"公理"和"实际应用"的分离,也许是认真的分析公理以及它们带来的问题在大部分量子力学研究中——甚至从数学物理的观点来看——明显不被关心的原因之一。

我们应该强调的是,Born, Heisenberg 的处理方法和 de Broglie, Schrödinger 的处理方法都扎根于互相关联的几个方面:对实验数据的关注、对早先理论的深刻理解、大胆的类比和近似,以及对"新力学"能否自圆其说的高度关注。

两种处理方法的出发点有着本质上的区别。在 Heisenberg 的处理方式中,原子并没有预先的空间结构;描述完全是依据它在光的发射和吸收下的性质,因此可观测量用矩阵来表示。动力学的进入是通过研究与电磁场的相互作用,以及一些与经典电动力学理论

在渐近区域的相似性(对应原理)。这样,正如我们已经简要指出的,一些矩阵的关系类似于 Hamilton 理论中位置和动量的关系。按照这种相似性,我们有可能将理论推广到最初的范畴之外,并且考虑电子不束缚在原子中的现象。

另一方面,在 Schrödinger 的处理方式中,粒子和粒子的集合用空间结构(波动)来表示。因此空间坐标是预先引入的,而且粒子的位置与相应的波的强度联系在一起(这是 Born 所强调的)。位置和动量都是经典力学中的基本可测量。物理解释迫使粒子的波动是平方可积的,数学则提供了同时对定域动量和位置的限制,这导致了 Heisenberg 的不确定性原理。动力学是从波粒二象性和与相对论波动方程在低能区域的相似性得到的。具有量子化能量的束缚态是众所周知事实——被限制在空间某个区域的波动的波数(因而能量)是量子化的——的结果。

形式结构

在这一节我们将描述与量子力学相关的形式数学结构。它由一个紧凑的数学理论组成,但是它所包含的诠释公理却导致了概念上的困难。

我们按照 J von Neumann(1966)的形式来陈述这些公理;它们由 Born, Heisenberg 和 Jordan 构造的形式理论的一个精确数学陈述组成。而 Schrödinger 形式本身不要求对可观测量的分类做出阐述。

公理 I

(i)可观测量用复的可分 Hilbert 空间 $\mathcal{H}$ 中的自伴算子表示。

(ii)每一个这样的算子都表示一个可观测量。

评注 公理 I(ii)只是为了数学上的简单性而引入的,对它并没有物理上的论据。原则上,一个可观测量必须与一种测量(观测)步骤相联系,而对于大部分 $\mathcal{H}$ 上的自伴算子(例如,Schrödinger 表象中的 $ix_k(\partial/\partial x_h)x_k$),这样的步骤并没有给出。

公理 II

(i)体系的纯态由 $\mathcal{H}$ 中归一化的矢量表示。

(ii)在用 $\phi\in\mathcal{H}$ 表示的状态中,对体系的可观测量 A 进行测量,得到的平均值则是一个实数$\langle\phi,A\phi\rangle$,这是因为 A 是自伴的(我们已经用$\langle\phi,\varphi\rangle$表示 $\mathcal{H}$ 中的内积)。

评注 注意公理 II 并没有对单次测量的结果做出表述。

利用 $\mathcal{B}(\mathcal{H})$的自然的复结构,纯态可以被推广为 $\mathcal{B}(\mathcal{H})$ 上的线性实泛函。

定义一个态作为 $\mathcal{B}(\mathcal{H})$(可分 Hilbert 空间 $\mathcal{H}$ 上的所有有界算子)上的任意线性的实的正泛函,如果它在强拓扑中是连续的,则称态是正规的。可以证明一个正规态能够被分解为一个由至多可数的纯态集合构成的凸组合。由这些定义,当且仅当一个态没有非平凡分解时,它是纯态。值得强调的是,只有对应于可观测量的算子可以生成整个 $\mathcal{B}(\mathcal{H})$ 时,这个表述才是正确的;人们通过不存在超选择定则这一表述来提及这个条件。

根据代数 $\mathcal{B}(\mathcal{H})$理论中的一般结果,一个正规态 ρ 由一个正定迹类算子通过公式 $\rho(A)=\mathrm{tr}(\sigma A)$来表示。因为正定的迹类算子(与经典对应物相似,通常称为密度矩阵)具有正的、总和为 1 的本征值 λ_k,正规态 ρ 的分解形式取为$\sigma=\sum_k\lambda_k\Pi_k$,其中 Π_k 是向第 k 个本征态投影的算子(多重计数)。

还可以很方便地知道,如果 $\mathcal{B}(\mathcal{H})$ 上的正规态 σ_k 的序列是弱收敛的(即对于每个 $A\in\mathcal{B}(\mathcal{H})$ 序列 $\sigma_k(A)$ 收敛),那么极限态是正规的。这个有用的结果对于 $\mathcal{B}(\mathcal{H})$ 的闭子代数一般是错误的,例如,对于没有最小投影的代数。

注意到,没有一个纯态对于所有的可观测量都是无色散的(与经典力学中发生的相反)。态 ρ_σ 对于可观测量 A 的色散定义为 $\Delta_\sigma(A)\equiv\sigma(A^2)-(\sigma(A))^2$。

态和与算子 A 相关的可观测量单次测量得到的结果之间的联系由下面的公理给出,我们将仅讨论只具有离散谱的自伴算子 A。对于其他情形的推广是直截了当的,但是需要利用 A 的谱投影。

公理Ⅲ

(i)如果 A 只有谱,则对 A 进行测量得到的可能结果是其本征值$\{a_k\}$。

(ii)如果体系在测量前的瞬间所处的状态用矢量 $\phi\in\mathcal{H}$ 表示,则测量得到结果 a_k 的概率是 $\sum_h|\langle\psi,\phi_h^{A;k}\rangle|$,其中 $\phi_h^{A;k}$ 是由本征值为 a_k 的本征矢量 A 张成的 Hilbert 空间中的完备正交集合。

(iii)如果体系处于纯态 ϕ 并且对可观测量 A 进行测量,并得到结果 $a_j\in(b-\delta,b+\delta)$,其中 $b,\delta\in R$,则在测量后的瞬间体系可以处于这样的任意态(不必要为纯态):它位于算子 A 在区间 $\Delta_{b;\delta}\equiv(b-\delta,b+\delta)$ 的谱子空间的纯态凸包中。

注意到,表述(ii)和(iii)可以被无修正地推广到初态不为纯态,而是用密度矩阵 σ 表示的情形。

评注 1 公理 III 确认了,如果在第一次测量后立即对同样的可观测量 A 进行进一步的测量,得到的结果将仍然位于区间 $\Delta_{b;\delta}$。这一点必须给予其结果所作的表述某种客观性;注意必须考虑"在……之后立即"的条件,因为体系的演化可能不会保持 A 的谱子空间的不变性。如果算子 A 在区间 $\Delta_{b;\delta}$ 只有离散谱(纯粹的点),可以将公理 III 用下面的方式表述:测量结果可以是任意的态,这个态可以被表示为本征值在 $\Delta_{b;\delta}$ 中的算子 A 的本征态的凸仿射叠加。

在非常特殊的情形,当 A 在 $\Delta_{b;\delta}$ 中只有一个本征值而且这个本征值不退化的时候,人们可以将公理 III 表述为如下的形式(通常称为"波包的塌缩"):体系在测量以后处于纯态,而且就是用算子 A 的一个本征态表示。

评注 2 注意第三公理做出了关于在测量完成后体系的状态的完全表述。

据公理 III,人们只能同时测量可交换的、用自伴算子表示的可观测量(即它们的谱投影是可交换的)。根据自伴算子的谱表示,交换算子构成的族$\{A_k\}$可以被考虑(即存在一个它们的表示)为共同测度空间中的函数。

公理 I~III 给出了量子力学的数学上自洽的理论形式,并且给出了对于任意可观测量的测量结果的统计描述(和统计预测)。值得注意的是,虽然预测只具有统计性,可观测量(及态)的动力学演化将由确定性的规律描写。预测所固有的统计性只是来自于第三个假定,它联系了理论的数学内容和测量过程。

第三公理虽然对于数学形式和实验数据的联系是至关重要的,但播下了折磨量子力学而且迄今没有治愈的概念困难的种子。

确实,第三公理说明,描述测量过程的规律本质上不同于支配无测量体系演化的规律。这种由测量效应造成之改变的特权角色导致了严重的概念上的困难,因为这种改变

和结果与是否被观测者记录是无关的;因此人们应该区分测量和与环境相互作用的差别。

一个根源于公理 III 的相关问题是,这个公理的表述隐含地牵涉一个鉴定测量结果的经典观测者的出现,他保证测量结果,且被允许使用经典的概率理论。因此这个观测者是不受量子力学的规律支配的。

概念上这两方面的困难有着它们共同的来源,这体现在将测量仪器与被测量的系统分割为满足不同规律的互不关联的实体。测量理论中的困难还没有得到一个满意的解答,但是人们已经做了各种各样的尝试,取得了不同程度的成功,它们其中的一些将在"诠释问题"这一节简要描述。因此目前形式的量子力学对于描述 Planck 尺度上的非相对论现象是一个精致和成功的理论,只是其内部一致性仍然建立在虚弱的基础上。

回到公理上来,值得注意的是,根据公理 II,一个态是可观测量的线性泛函,但是它用复 Hilbert 空间 $\mathcal{H}$ 上的半双线性函数表示。因为公理 II 规定 $\mathcal{H}$ 中任意归一化的元素表示一个态(并且仅差一个相位的元素表示相同的态),考虑 ϕ 和 ψ,那么 $\xi \equiv a\phi + b\psi$,$|a|^2 + |b|^2 = 1$ 表示态 ϕ 和 ψ 的叠加态(叠加原理)。

但是对于一个可观测量 A,由于内积中的交叉项,我们一般有 $\rho_\xi(A) \neq |a|^2\rho_\phi(A) + |b|^2\rho_\psi(A)$。叠加原理是量子力学的一个典型特征。两个纯态 ϕ 和 ψ 的叠加具有完全不同于由密度矩阵 $\sigma = |a|^2\Pi_\phi + |b|^2\Pi_\psi$ 定义的这两个态的统计混合的性质,这里我们已经用 Π_ϕ 表示向归一化矢量 ϕ 的正交投影。所以,寻找这些干涉项是检验量子力学预言的一种方式,并且在给定条件下它们的值很小是所研究的体系具有半经典行为的标志。

与叠加原理紧密相关的是纠缠和部分求迹操作。假设我们有两个系统,分别考虑的时候用两个 Hilbert 空间 $\mathcal{H}_i$,$i = 1, 2$ 中的矢量来描写,它们具有可观测量 $A_i \in \mathcal{B}(\mathcal{H}_i)$。当我们想要研究它们之间的相互作用时,很自然地要在 Hilbert 空间 $\mathcal{H}_1 \otimes \mathcal{H}_2$ 中描述两者,而且考虑可观测量 $A_1 \otimes I$ 和 $I \otimes A_2$。

当系统相互作用的时候,相互作用与 $\mathcal{H}_1$ 上的投影算符 Π_1 一般不对易。所以,即使初态是 $\phi_1 \otimes \phi_2$,$\phi_i \in \mathcal{H}_i$ 的形式,(相互作用后的)末态是一个矢量 $\xi \in \mathcal{H}_1 \otimes \mathcal{H}_2$,它不能写成 $\xi = \zeta_1 \otimes \zeta_2$,其中 $\zeta_i \in \mathcal{H}_i$。然而,可以证明,总是存在两族正交归一的矢量 $\phi_n \in \mathcal{H}_1$ 和 $\psi_n \in \mathcal{H}_2$,使得对于合适的 $c_n \in C$,$\sum |c_n|^2 = 1$,有 $\xi = \sum c_n \phi_n \otimes \psi_n$(这个分解一般是不惟一的)。

注意到 $\rho_{\phi\otimes\psi}(A_1 \otimes I) = \rho_\phi(A_1)$,可以写出

$$\rho_\xi(A_1 \otimes I) = \sum |c_n|^2 \rho_{\phi_n}{}^{①}(A_1) = \rho_{\sigma_1}{}^{②}(A_1)$$

$$\sigma_1{}^{③} \equiv \sum_n |c_n|^2 \Pi_{\phi_n}$$

映射 $\Gamma_2 : \rho_\xi \to \rho_{\sigma_1}$ 称为相对于 $\mathcal{H}_2$ 的约化;它也称为相对于 $\mathcal{H}_2$ 的"部分求迹"。反映了与经典概率理论中条件作用④的相似性。

由线性性质,映射 Γ_2 可以被推广到从 $\mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ 上的正规态(密度矩阵)到 $\mathcal{B}(\mathcal{H}_1)$ 上的正规态的映射,并给出一个保持正定性和保持迹不变的映射。

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① 应为 ρ_{ϕ_n},而不是 ρ_{ξ_n},原文有误 — 译者注。

②,③ 应为 σ_1 而不是 σ,原文有误 — 译者注。

④ 即概率论中的条件期望 — 译者注。

事实上可以证明(Takesaki 1971),在 $\mathcal{MB}(\mathcal{K})$ 张量化后保持正定的意义下,对 von Neumann 代数 $\mathcal{M}$ 的正规态的任意条件作用是完全正定的,其中 $\mathcal{K}$ 是任意的 Hilbert 空间。

我们也可以证明部分的逆命题为真,也就是说,对于合适选择的一个更大的 Hilbert 空间 $\mathcal{K}$ 和部分等距 V_k,作用在 von Neumann 代数 $A\in\mathcal{B}(\mathcal{H})$ 的正规态上的每一个完全正定的保持迹不变的映射 Φ 可以被写成 $\Phi(a)=\sum_k V_k^* a V_k$ 的形式(Kraus 形式)。

但是必须指出的是,如果 $U(t)$ 是 $\mathcal{H}_1\otimes\mathcal{H}_2$ 上的酉算子构成的单参数群且 σ 是密度矩阵,则映射 $\Gamma(t)\equiv\sigma\to\Gamma_2(U(t)\sigma U^*(t))$ 的单参数族一般不具有半群的性质 $\Gamma(t+s)=\Gamma(t)\cdot\Gamma(s)(s,t>0)$,因而一般不存在与它相联系的(约化动力学的)生成元。只有在特殊情形和非常强的假设和近似下,存在一个由(Markov 性质)半群给出的约化动力学。

因为纠缠和(非平凡的)条件作用是量子力学的标志,而另一方面上面所描述的 Markov 性质是经典力学中典型的条件作用,所以人们很自然的要探求在什么条件和近似下 Markov 性质得到恢复,并且更一般性的,在何种条件和近似下作为量子力学特征的相干性质得到压制(退相干)。我们将在"诠释问题"这一节中简要讨论这个问题,用以尝试克服由公理 III 遗留下来的严重的概念上的困难。

从上面的评注和定义中看到,正规态(密度矩阵)扮演了经典力学相空间中测度的角色。一个例外是,量子力学中的纯态并不对应于 Dirac 测度(稍后我们将讨论用相空间中的函数(Wigner 函数)描写量子力学态的可能性)。

在这样的对应中,在一个态(归一化,正测度)计算一个可观测量(相空间上一个可测函数)是与找出一个 $\mathcal{B}(\mathcal{H})$ 中的算子与一个密度矩阵乘积的(在 Hilbert 空间的)迹相联系的。注意求迹运算有一些与积分相同的性质,特别是,如果 A 在迹类中而且 $B\in\mathcal{B}(\mathcal{H})$(比较 $g\in L^1$ 和 $f\in L^\infty$)$\mathrm{tr}(AB)=\mathrm{tr}(BA)$,以及如果 A 是密度矩阵而 B 是正定算符,那么 $\mathrm{tr}(AB)>0$。这建议我们定义在密度矩阵上的函数,它们对应于动力学系统尤其是熵理论中重要的量。

这很容易做到,条件是 Hilbert 空间是有限维的,以及在无限维的情形人们取所有的 Hermit 有界算子为可观测量。在量子统计力学中人们被引导到考虑无限多个子系统的集合,每一个由一个 Hilbert 空间(有限或者无限维)$\mathcal{H}_i$,$i=1,2,\cdots$ 描写,表示空间是 $\mathcal{H}_1\otimes\mathcal{H}_2\otimes\cdots$ 的一个子空间 $\mathcal{K}$,可观测量是 $\mathcal{B}(\mathcal{K})$ 的一个(弱闭)的子代数 $\mathcal{A}$(典型的构造是一个形式为 $I\otimes I\otimes\cdots\otimes A_k\otimes I\otimes\cdots$ 的元素的归纳极限)。我们也考虑 $\mathcal{A}$ 上的正规态并定义一个求迹运算,求迹具有上面描述的性质。大部分的定义(例如,熵)可以在更大的背景中给出,但是差别可能会出现,因为一般来说 $\mathcal{A}$ 并不包含有限维的投影,因此求迹函数并不是通常的定义在 Hilbert 空间上的求迹运算。我们将不再进一步描述这个非常有趣而且发展很快的理论,它主要与量子统计力学相关。一个彻底的描述可以参看 Ohya 和 Petz (1993)。

最简单且被广泛研究的例子是每个 Hilbert 空间 $\mathcal{H}_i$ 都是二维复空间的情形。构建出的系统与经典统计力学中的 Ising 模型类似。不同的是,对于指标 i 的每一个值它都拥有无穷多的纯态。相应的可观测量的代数是 $(C^2\times C^2)^{\otimes Z}$ 的一个闭的子代数,并且一般不包含任何有限维的投影。

如果限制在$(C^2\times C^2)^K$的情形,其中K是有限整数,这个模型在量子信息和量子计算研究中已经很流行。在这种情形中,$\mathcal{H}_i$的一个归一化的元素被称为一个q比特(与经典信息理论中信息的比特类似)。很清楚的是,$(C^2\times C^2)$中的单位圆包含了远多于4个的点,这给出了对系统操作的更多自由度。这就是量子信息和量子计算——一个近年来得到很多关注的非常有趣的领域——的基础。

量子化与动力学

在非相对论量子力学中,时间演化由Hilbert空间中的Schrödinger方程描述。对于含N个粒子的系统,Hilbert空间是$L^2(R^{3N}\otimes C^k)$,其中引入有限维空间C^k是考虑到有些粒子具有自旋自由度这一事实。

除一些通常的非本质的参量之外,典型的自旋0粒子的Schrödinger方程可写成

$$i\hbar\frac{\partial\phi}{\partial t}=H\phi$$

$$H\equiv\sum_{k=1}^{N}m_k(i\hbar\nabla_k+A_k)^2+\sum_{k=1}^{N}V_k(x_k)+\sum_{i\neq k,1}^{N}V_{i.k}(x_i-x_k)\qquad[9]$$

式中,$\hbar$是Planck常数,A_k是R^3上的矢量函数(矢量势),V_k和$V_{i.k}$是R^3上的标量函数(标量势)。

如果有些粒子的自旋是1/2,那么相应的动能项应为$-(i\hbar\sigma\cdot\nabla)^2$,其中$\sigma_k,k=1,2,3$是Pauli矩阵。另外还必须加入势能项$W(x)$,它应为取值在$C^k\otimes C^k$中的矩阵场,并考虑自旋自由度之间的相互作用。注意,局部算子$i\sigma\cdot\nabla$是拉普拉斯算子的一个"平方根"。

三维空间中质量$m\geqslant 0$的自由粒子的Schrödinger方程的相对论推广是由Dirac得到的。推广后的方程定义在由旋量函数$\psi_k(x,t),k=0,1,2,3$构成的空间中,这些函数携带着Lorentz群的一种不可约表示。类似电磁场情况,那里一个线性偏微分方程(PDE)可以用Lorentz群的四维表示写出来,相对论性Dirac方程也是线性偏微分方程

$$i\sum_{k=0}^{3}\gamma_k\frac{\partial}{\partial x_k}\psi=m\psi,\quad x_0\equiv ct$$

式中,γ_k生成Lorentz群的一个表示代数。算子$\sum(\partial/\partial x_k)\gamma_k$是相对论不变d'Alembert算子$-\partial^2/\partial x_0^2+\nabla-m\cdot I$的一个局部平方根。

当人们试图引入(相对论不变的)定域相互作用时,面对和在经典力学中一样的问题,即人们必须引入相对论协变场(例如电磁场),也就是具有无穷多自由度的系统。如果这种场是作为外源考虑的,人们面对的是一些技术问题,顺利的情况下是可以解决的。但如果人们试图得到一个完全量子化的理论(通过场量子化),会遇到不可克服的困难,部分是由于技术上的,部分是由于正则交换关系的不惟一性,如果这些关系被用来作为量子化的基础。其情形就像在有限维时那样。

在某些顺利的情况下(例如,量子粒子与量子化的电磁场相互作用),人们可以建立对于某参数α的微扰论(自然单位制下α的物理值大约是1/137)。我们稍后在讨论Schrödinger算子时会回到微扰论上来,现在的情况是人们已经能找到一些(重整化)手续使得描述相应物理问题的α展开级数是一级接一级地良好定义的。但就算在这种顺利的情况下——这时级数的前几项之和可以极好地与实验数据吻合,人们还是有理由相信级

数是不收敛的,甚至人们不知道级数是否是渐近的。

人们想知道场(在经典时空上紧致光滑函数之对偶空间中的算子值元素)的结构——它们是从经典的电磁学简单地继承过来的,在描述发生在比原子尺度还要小得多的尺度上的现象时是否还是一种有效的手段。而我们有理由相信原子尺度上发生的自然现象可以用 Schrödinger 和 Heisenberg 提供的方法来描述。

与量子化的非相对论粒子和量子化的电磁场之间的相互作用有关的现象是发生在原子尺度上的。这些现象已经是理论物理中广泛研究的课题,大多数的研究是在微扰论的框架下,对于前几阶的分析就已经导致非常引人注目的结果(尽管现在还没有证明微扰级数至少是渐近的)。

这一领域中的严格解很少,但近年来也有所进展。譬如证明了基态的存在性(这是一个非平凡的结果,因为没有能隙分开基态和谱的连续部分)并且为描述散射现象铺平了道路;后者也是非平凡的因为光子场可能导致反常的红外(长程)行为,所以非相对论散射理论中长程 Coulomb 相互作用需要特别的处理。

本文作为百科全书中的一篇,旨在给量子力学一个介绍,因而我们将只考虑非相对论理论的基本结构。非相对论性量子理论处理有限数目的粒子间相互作用以及它们与(经典)外势场的作用。关于量子力学的高级论题以及量子粒子与量子场间的相对论不变相互作用理论的成功与失败之处将留给专门的条目去讨论。

我们回到基础上来。

我们可以通过讨论 Schrödinger 方程解的性质来研究量子力学的动力学。包括色散效应以及相关的散射理论,束缚态与共振态的问题,含时微扰与电离(离解)效应,原子与分子的束缚,Rayleigh 散射,Hall 效应以及其他纳米物理效应,各种多尺度和绝热极限,以及所有通过成功求解 Schrödinger 量子力学来解决的物理问题(以及也还有大量有趣但未解决的问题)。

我们只简要地讨论这些课题以及为了对那些人们感兴趣的物理量做明确的估计而发展的近似方法。已经有大量优秀的综述性文章讲述当前量子力学的研究状况(例如,Araki 和 Ezawa (2004),Blanchard 和 Dell'Antonio (2004),Cycon 等人(1986),Islop 和 Sigal(1996),Lieb(1990),Le Bris(2005),Simon(2002),以及 Schlag(2004)),我们希望读者通过查阅本百科全书的专门条目来获得关于这些结果的具体分析和准确陈述。

我们先回到理论的基础部分;我们将采用 Heisenberg 的观点,并且从讨论观察量代数和态代数的映射性质开始。由于跃迁概率扮演重要的角色,我们只考虑这样的变换 α:对于任何一对纯态 ϕ_1 和 ϕ_2,它们满足 $\langle \alpha(\phi_1), \alpha(\phi_2)\rangle = \langle \phi_1, \phi_2\rangle$。我们称这样的映射为 Wigner 自同构。

Wigner 的一个结果(见 Weyl(1931))称,如果 α 是一个 Wigner 自同构,那么存在惟一的算子 U_α,它要么酉要么反酉,使得对所有投影算子 P 有 $\alpha(P) = U_\alpha^* P U_\alpha$。如果有这样的自同构的一个单参数群,那么相应的算子都是酉的(但它们不需要构成一个群)。

这个结果的一个推广是 Kadison 得到的。用 $\boldsymbol{I}_{1,+}$ 表示密度矩阵集合,按照定义,对于所有 $\sigma_1, \sigma_2 \in \boldsymbol{I}_{1,+}$ 与 $0<s<1$,一个 Kadison 自同构 β 有 $\beta(s\sigma_1 + (1-s)\sigma_2) = s\beta(\sigma_1) + (1-s)\beta(\sigma_2)$。Kadison 自同构有和 Wigner 自同构一样的结果。

类似的结果对于观察量的自同构也成立。注意两个 Hermit 算子的乘积一般不再是

Hermit 算子,但 Hermit 在 Jordan 积下是保持的,Jordan 积定义为 $A\times B\equiv(1/2)[AB+BA]$。

一个 Segal 自同构,按定义,是一个保持 Jordan 积结构的 Hermit 算子自同构。由 Segal 的一个定理,γ 是一个 Segal 自同构,当且仅当存在一个正交算子 E,$E\mathcal{H}$ 中的一个酉算子 U 和 $(\boldsymbol{I}-\boldsymbol{E})\mathcal{H}$ 中的一个反酉算子 V 满足 $\gamma(A)=WAW^*$,其中 $W\equiv U\oplus V$。

利用态的 Wigner 或 Kadison 自同构和对于观察量的 Segal 自同构,我们可以更具体地描述动力学。我们要求在合适的拓扑下,时间演化是连续的。最好的结果是在 Wigner 情形。可以证明,如果 Wigner 自同构 α_t 的一个单参数群在弱拓扑下是可测的(即对任何 A 和 σ,$\alpha_t\sigma(A)$ 对 t 是可测的),那么可以选择 Wigner 定理中的 $U(t)$ 使得它们可以构成群,且该群在强拓扑下是连续的。对 Kadison 和 Segal 自同构情形也有相似的结果,但这时必须假定 α_t 是强拓扑意义下连续的(对 Segal 情形是强算子拓扑,对 Kadison 情形是范数拓扑)。如果算子乘积是保持的,则只需要弱连续性的条件(这种情况下要考虑有界算子代数的自同构)。连续群 $U(t)$ 的存在性定义了一个哈密顿演化。确实,我们有

定理 1(Stone) 当且仅当在 $\mathcal{H}$(中的一个稠密子集)上存在一个自伴算子 H,满足 $U(t)=e^{itH}$,映射 $t\to U(t)$,$t\in R$ 是在 Hilbert 空间 $\mathcal{H}$ 中的酉算子集中 R 的一个弱连续表示。因此有

$$\phi\in D(H)\to i\frac{\mathrm{d}U(t)}{\mathrm{d}t}\phi=HU(t)\phi \qquad [10]$$

算子 H 称作由 $U(t)$ 描述的动力学的生成元。

注意:在 Schrödinger 方案中,Stone 定理中所描述的算符称作哈密顿量,和经典力学相似。R^3 中质量为 m 的粒子在具有势 $V(x)$ 的时保守力作用下时,体系的哈密顿量具有如下形式($\hbar=1$):

$$H=-\frac{1}{2m}\Delta+V(x),\Delta=\sum_k\frac{\partial^2_{x_k}}{\partial x_k^2} \qquad [11]$$

如果势 V 依赖于时间,Stone 定理不能直接使用,这时自伴算子 H_t 的谱性质和群 $\tau\to e^{iH_t\tau}$ 核的谱性质对于求解(时间依赖)的 Schrödinger 方程是关键的。

半群 $t\to e^{-tH_0}$① 通常是收缩的保正性半群,并且定义了一个 Markov 过程;在好的情况下对 $t\to e^{-tH}$ 也有相同的结果(Feynmann-Kac 公式)。

对于 von Neumann 代数上的动力系统的一般理论也有类似的情形;类似于椭圆算子,我们定义 von Neumann 代数 $\mathcal{M}$ 上的"耗散"映射 Δ 为它满足 $\Delta(a*a)\geqslant a^*\Delta(a)+\Delta(a^*)a$,$a\in\mathcal{M}$。正耗散 Δ 称作完全正的,如果它对于任何 Hilbert 空间 $\mathcal{K}$ 而言 $\mathcal{MB}(\mathcal{K})$ 的张量化保持为正。注意,根据该定义,每个 *-导数都是完全正耗散的。对于耗散(算子)有一个类似 Stinespring 定理的结果,且通常有界耗散(算子)可写为

$$\Delta(a)=i[h,a]+\sum V_k^*aV_k-\frac{1}{2}\sum\{V_k^*V_k,a\},a\in\mathcal{M}$$

(符号{.,.}表示反交换子)。

一般说来,所谓量子化是指通过将经典相空间 X 上函数的交换代数变形来构造一个

① 这里 $H_0=\frac{1}{2m}\Delta$——译者注。

理论使得量子系统的动力学能从形变的规则中导出来,如果 X 是余切丛 $T^*\mathcal{M}$[①],那么通常就将泊松括号变形(Halbut 2002,Landsman 2002)。我们将只讨论 Weyl 量子化(weyl 1931),它是量子力学 Heisenberg 形式的基础,并且与构形空间是 R^N 或 N 维圆环面(Floquet-Zak)的情形相关。我们将对 Wick(反 Weyl)量子化稍做评述。如果试图量子化一个定义在一般余切丛或甚至一般辛流形上的经典系统时,需要更加一般的量子化形式。

Weyl 量子化是对 Born 和 Heisenberg 方案的核心内容的精确数学表述。后者是通过寻找扮演辛坐标角色的算子来构造动力学的。

考虑一个单自由度系统。最简单的尝试是寻找算符$\hat{q}$,$\hat{p}$使得如下关系成立

$$[\hat{q},\hat{p}]\subset i\boldsymbol{I} \qquad [12]$$

然后仿照经典情况来构造哈密顿量。为了能扮演类似经典情况下的角色,算子$\hat{q}$,$\hat{p}$必须是自伴的且至少在不太严格的意义下满足式[12]。如果$\hat{q}$,$\hat{p}$都是有界的,式[12]导致$e^{-i\hbar\hat{p}}\hat{q}e^{i\hbar\hat{p}}=\hat{q}+b\boldsymbol{I}$(指数是通过收敛级数来定义的),从而$\hat{q}$的谱将是整个实轴,这是互相矛盾的结果。因此,式[12]中的包含符号是严格的,并且我们面对定义域的问题,结果是式[12]有很多不等价的解("等价"是指"酉等价")。

除了一些"病态"的解外,式[12]有定义在 R 的多重覆叠[②]上的 L^2 空间中不等价解,它们被有效地应用于量子力学中。

最常见的解定义于 Hilbert 空间 $L^2(R)$中(在 Lebesgue 测度下)。这时$\hat{x}$被定义为自伴算子,它作用在紧致光滑函数上就是用坐标 x 乘以该函数;$\hat{p}$被类似地定义在 Fourier 空间中。这种表示可以简单地推广到 $L^2(R^N)$情况下来构造$\hat{q}_k$ 和$\hat{p}_k$。

式[12]的另一个经常使用的表示是在空间 $L^2(S^1)$中(当推广到 N 自由度时,空间为 T^N)。在这种表示中,算子$\hat{p}$对函数 $f(\theta)=\sum_{k=-M}^{N}c_k e^{ik\theta/2\pi}$,$0\leqslant M,N<\infty$ 的作用由 $c_k\to kc_k$ 来定义。算子$\hat{q}$定义为对该函数乘以角坐标 θ。容易验证这种表示与前一种表示是不等价的,式[12]在$\hat{q}\,\hat{p}$和$\hat{p}\,\hat{q}$的共同定义域的(稠密)矢量集合中是(作为恒等式)满足的。但注意,算子$\hat{p}$的本性自伴域在$\hat{q}$的作用下不是左不变的(只有当 $f(2\pi)=0$ 时 $\theta f(\theta)$是 S^1 上的函数)。

在该表示中,我们将用$\partial/\partial\theta_{\text{per}}$来标记$\hat{p}$并把它称作 Block 表示。可以把$\hat{p}$对函数的作用修改为 $c_n\to nc_n+\alpha$,$0<\alpha<2\pi$,这样就给出各种 Bloch-Zak 表示和磁表示。

注意到 $L^2(R)=L^2(S^1)\otimes l^2(N)$,Bloch 表示可被扩展到 R^1 上的周期函数;同样,Bloch-Zak 表示和磁表示也可以扩展到 $L^2(R^N)$。

表示之间的差别可以通过考虑由"典则算子"$\hat{p}$,$\hat{q}$生成的酉算子的单参数群看得更清楚。在 $L^2(R)$的 Schrödinger 表象中,这些群满足

$$U(a)V(b)=e^{iab}V(b)U(a),U(a)=e^{ia\hat{q}},V(b)=e^{ib\hat{p}}$$

因此,令 $z=a+ib$,$W(z)=e^{-iab/2}V(b)U(a)$,有

$$W(z)W(z')=e^{-i\omega(z,z')/2}W(z+z'),z\in C,\omega(z,z')=Im(\bar{z},z') \qquad [13]$$

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① 这里应为 $T^*\mathcal{M}$,而 $\mathcal{M}$ 为微分流形——译者注。

② 此处有误,应为圆环 S^1 多重覆叠——译者注。

酉算子 $W(z)$因而是加群 C 的投影表示。推广到 N 自由度情况是直接的;表示现在具有加群 C^N,ω 就是 C^N 上的标准辛形式。

在 Bloch 表示中,$U(a)V(b)U^*(a)V^*(b)$不是恒等元的倍数,并且没有特别简单的形式。带有结构式[13]的映射 $C^N \ni z \to W(z)$称作 Weyl 系统;它在量子力学中扮演主要的角色。因此下面的定理在量子力学的数学理论中特别重要。

定理 2(von Neumann 1965) Weyl[①] *系统存在惟一(除去酉等价)的不可约表示。*

该定理的证明可采取群表示论的一般步骤。引入由算子

$$W_f \equiv \int f(z)W(z)\mathrm{d}z, f \in L^1(C^N)$$

组成的 Weyl 代数 $\mathcal{W}^{(N)}$。

容易看出 $|W_f| = |f|_1$,如果将具有自然乘积结构的 $\mathcal{W}^{(N)}$ 和 L^1 看成具有乘积结构

$$f * g \equiv \int \mathrm{d}z' f(z-z')g(z')\exp\frac{i}{2}\omega(z,z') \qquad [14]$$

的非交换代数,则 $f \to W_f$ 是代数的一个线性同构。至此 $\mathcal{W}^{(N)}$ 是 $L^2(R^2)$上有界算子的具体代数。但它也可看作一个抽象 C^* 代数,我们依然记它为 $\mathcal{W}^{(N)}$。

容易看出,按照式[14],如果选择 f_0 为一个合适的高斯分布,那么 W_{f_0} 是一个与所有 W_f 可交换的投影算子。并且,$W_fW_g = \phi_{f,g}W_{f*g}$,$\phi$ 是一合适的相因子。考虑到 C^* 代数 $\mathcal{W}^{(N)}$ 的 Gelfand-Neumark-Segal 构造,那么这些性质导致在循环不可约等价类中任一表示的分解,从而完成定理的证明。

Weyl 系统有一个在空间 $L^2(R^N, g)$中的表示(等价于 Schrödinger 表示),这里 g 是高斯测度。由此可以做一个延拓,将 C^N 替换为一个具备高斯测度(弱分布(Segal 1965, Gross 1972, Wiener 1938))的无穷维 Banach 空间。在此更一般的框架下,惟一性失效(惟一性与 C^N 中单位球的紧致性严格相关)。在 Schrödinger 表象下(因而,在任何表象下),谐振子的哈密顿量定义了一个正自伴算子

$$N = \sum_1^N N_k, N_k = -\frac{\partial}{\partial x_k^2} + x_k^2 - 1$$

可交换的算子 N_k 中的任意一个的谱由正整数(包括 0)组成,因而称作第 k 个自由度的数算子。算子 N_k 可以写成 $N_k = a_k^* a_k$,其中 $a_k = (1/\sqrt{2}(x_k + \partial/\partial x_k))$,$a_k^*$ 是 a_k 在 $L^2(R)$中的形式对偶。我们有 $|a_k(N_k+1)^{-1/2}| < 1$。在 N 的定义域中,这些算子满足如下的关系(典则交换关系)

$$[a_k, a_l^*] = \delta_{k,l}, [a_k, a_l] = 0, [N_k, a_l] = -a_l\delta_{k,l}, [N_k, a_l^*] = a_k^*\delta_{k,l} \qquad [15]$$

通过观察最后两个关系,算子 a_k 可以称作湮灭算子(对第 k 个自由度),它的形式对偶称作产生算子。算子 a_k 的谱为整个复平面,算子 a_k^* 的谱为空集;N_k 的本征矢是变量 x_k 的 Hermite 多项式。a_k 的本征矢(即 $L^2(R)$中方程 $a_k\phi_\lambda = \lambda\phi_\lambda$,$\lambda \in C$ 的解)叫相干态;它们在 Bargmann-Fock-Segal 量子化和一般的半经典极限中扮演主要角色。

算子集$\{N_k\}$生成一个最大阿贝尔系统,所以空间 $L^2(R^N)$有一个作为$\oplus_k (C^N)^k$的对称化子空间的自然表示(Fock 表示)。该表示中,算符 N_k 的共同本征矢 ϕ_{n_k},$k = 1, \cdots, N$

① 原文误为 weil——译者注。

构成一个自然基。一般的矢量可以写作

$$\psi = \sum_{n_k} c_{n_k} \phi_{n_k}, \sum_{n_k} |c_{n_k}|^2 < \infty$$

因而可用序列 c_{n_k} 表示。

注意,产生算符不会在 R^N 中产生粒子,而是使 Hermite 多项式组成的基之间产生转移。

习惯用 $\gamma(L^2(R^N))$标记 Fock 表示(也叫二次量子化,因为对每个自由度,波函数是在谐振子的量子化的基上写出的),用 $\Gamma(\boldsymbol{A})$表示矩阵 $\boldsymbol{A} \in \boldsymbol{B}(C^N)$的提升。如 C^N 被 Banach 空间 X 代替,这些记号是特别有用的。这些术语是由 Segal 在他的关于波方程量子化的工作中引入的,并且从那以后就被使用,特别是在微扰论中。

在量子场论中,空间 C^N 被替换为函数的 Banach 空间 X。在此框架内,"二次量子化"(Segal 1965,Nelson 1974)把态 ϕ_{n_k} 看成系统中恰好有 n_k 个粒子处于第 k 个物理态(前提是已经选择了 R^3 中分布空间的一组基)的构形。这样做没有任何问题(Gross 1972),如果希望在 X 中合适的内积$\langle .,. \rangle$下,交换关系式[16]的推广可以写成$[a^*(f), a(g)] = \langle f, g \rangle$,则可以选一合适的 Sobolev 空间(它依赖于在 X 中给定的高斯测度)。相对论场量子化的问题是,为了保证定域性,我们被迫使用带负指标(依赖于物理空间的维数)的 Sobolev 空间,这在定义非线性矢量场的动力学时导致困难。

注意,在 Segal(1965)的工作以及后来的构造场论(Nelson 1974)中,Fock 表示被置于 Schrödinger 框架中,这时相关的算子作用于空间 $L^2(X, g)$上,其中 X 是我们想要描述的粒子所在的物理空间的 Schwarz 分布空间的一个子空间,g 是适当地定义在 X 上的高斯测度。

Fock 表示与 Bargmann-Fock-Segal 表示有关(Bargmann 1967),后者是在 C^N 上高斯测度平方可积的全纯函数构成的空间中的一个表示。

Fock 表示的发展在历史上依赖特普刊兹算子和陶伯估计的性质。它被大量用于半经典极限的研究和经典相空间不是余切丛(例如,二维球)系统的量子力学描述。

评注 无穷维 Weyl 系统的 Fock 表示只能描述服从 Bose-Einstein 统计的粒子;确实,态受到在所选择的基中被描述粒子的限制,区分一个 N 粒子态中的每个粒子是不可能的。在有限维情形这是明显的:二阶 Hermite 多项式不能看作是两个一阶多项式的组合。

在无穷维情况下,如果要处理服从 Fermi-Dirac 统计的粒子就必须依赖 Pauli 不相容原理(Pauli 1928)。由该原理,两个这样的粒子不能处于同一个构形中;为了保证这一点,波函数必须在置换粒子记号时是反对称的。有如下事实(相对论量子场论中的一个定理,是理论的协变性,定域性和能量正定性的结果(Streater, Wightman(1964))),半整数自旋的粒子服从 Fermi-Dirac 统计。所以,要量子化这样的系统,就必须引入与 Weyl 系统不同的(对易)关系。因为现在反对称性导致$(a^*)^2 = 0$,引入下列关系将是合理的(典则反交换关系):

$$\{a_k, a_l^*\} = \delta_{k,l}, \{a_k, a_l\} = 0, \{N_k, a_l\} = -a_l \delta_{k,l}, \{\boldsymbol{A}, \boldsymbol{B}\} = \boldsymbol{AB} - \boldsymbol{BA} \quad [16]$$

Hilbert 空间是$\otimes^N \mathcal{H}_2$,其中 $\mathcal{H}_2$ 是一个二维复 Hilbert 空间。注意,$\mathcal{H}_2$ 携带有 $SU(2) \equiv O(3)$的一个二维不可约表示(自旋表示),所以这种量子化把 1/2 自旋和反交换性关联起

来。

式[16]中的算子都是有界的(事实上在范数意义下以 1 为界)。Fock 表示可以像在 Weyl 情形时那样构造出来((见 Araki(1988)),但对每个指标 k,n_k 等于 0 或 1。无穷维情况以同样的方法定义,并得到不等价不可约表示(Araki 1988);但只有其中一个表示可以定义数算符并是下有界的。如果引入规范及基于迹的积分形式(Gross 1972),某些表示可以给出类 Schrödinger 形式。这种系统多用于量子统计力学中,因为它处理有界算符且可以利用 C^* 代数中一些很强的结果。在无穷维情况(偶尔对一般情况)它被用于量子信息(空间 $\mathcal{H}_2$ 是量子比特空间)。

回到 Weyl 系统,我们现在引入与其严格相关的 Wigner 函数。后者在半经典极限的分析和一些标度极限的讨论中扮演重要角色,特别是流体力学极限和 $N\to\infty$时的 Bose-Einstein 凝聚。

纯态 ϕ 的 Wigner 函数 W_ϕ 是经典系统的相空间中的实值函数,它忠实地表示态 ϕ。它的定义是

$$W_\phi(x,\xi) = (2\pi)^{-n}\int_{R^n} \mathrm{e}^{-i(\xi,x)}\phi\left(x+\frac{y}{2}\right)\bar{\phi}\left(x-\frac{y}{2}\right)\mathrm{d}y$$

Wigner 函数一般不是正的(惟一的例外是满足 $\Delta(x)\cdot\Delta(p)\geqslant\hbar$ 的高斯态)。但它有有趣的性质,它的边缘性可以正确地导出 Born 规则。事实上有 $\int W_\phi(x,\xi)\mathrm{d}x = |\hat{\phi}(\xi)|^2$。如果函数 $\phi(t,x)$,$x\in R^n$ 是自由 Schrödinger 方程 $i\hbar\partial\phi/\partial t=-\hbar^2\Delta$ 的解,那么其 Wigner 函数满足 Liouville(输运)方程$\partial W_\phi/\partial t+\xi\cdot\nabla W=0$。

Wigner 函数与 Weyl 量子化关系密切。weyl 量子化给一个给定正规类里的函数 $\sigma(p,x)$关联一个算子 $\sigma(D,x)$(函数 σ 的 Weyl 符号)

$$(\sigma(D,x)f,g) = \int\sigma(\xi,x)W(f)(\xi,x)\bar{g}(\xi,x)^{①}(\xi,x)\mathrm{d}\xi\mathrm{d}x,$$

$$W(f)^{②}(\xi,x) = \int \mathrm{e}^{-i(\xi,p)}f\left(x+\frac{p}{2},x-\frac{p}{2}\right)\mathrm{d}p$$

可以验证,$F^{③}$ 的作用保持 Schwartz 类 S 和 S'并在 $L^2(R^{2N})$中是酉的。而且,有 $\sigma(D,x)^*=\bar{\sigma}(D,x)$。

Weyl 量子化与 Wigner 函数之间的关系容易从有界算符和纯态之间的自然对偶看出来:

$$\mathrm{tr}(\hat{A}\hat{\rho}) = \int a(p,q)\rho(p,q)\mathrm{d}p\mathrm{d}q,\rho(p,q) = \int e^{i(p,q')}\rho(q',q)\mathrm{d}q'$$

我们现在简单讨论一下量子化的一般结构,然后把它用到 Weyl 量子化上。所谓将一个哈密顿系统量子化是指经典可观察量(相空间 $\mathcal{F}$ 上的实函数)与量子可观察量(*Hilbert* 空间 $\mathcal{H}$ 上的自伴算子)之间的一种对应,该对应可以用一小量 $\hbar$ 来参数化,并且有如下性质,在极限 $\hbar\to0$ 时两种观察量的结构是一致的,在$\hbar\neq0$ 时它们之间的差别可以在合适的拓扑下估计出来。

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① 原文误为 $W(f,g)(\xi,x)$— 译者注。

② 原文误为 $W(f,g)$—— 译者注。

③ F 指傅里叶变换——译者注。

最后的这条要求在应用时是重要的,从这个观点看,Weyl 量子化比其他量子化形式给出更强的结果。

我们只讨论 $\mathcal{F}=T^*X, X\equiv R^N$ 的情况,并且用 $L^2(R^N)$ 来实现 $\mathcal{H}$。

令 $\{x_i\}$ 是 R^N 的笛卡儿坐标,考虑一个满足如下要求的对应 $A\to\hat{A}$:

(1)$A\leftrightarrow\hat{A}$ 是线性的;

(2)$x_k\leftrightarrow\hat{x}_k$,其中 $\hat{x}_k$ 是乘以 x_k 的运算;

(3)$p_k\leftrightarrow i\hbar\partial/\partial x_k$;

(4)若 f 是 R^N 中的连续函数,那么 $f(x)\leftrightarrow f(\hat{x})$,$\hat{f}(p)\leftrightarrow(Ff)(\hat{x})$,其中 F 表示傅里叶变换;

(5)$L_\zeta\leftrightarrow\hat{L}_\zeta$,$\xi\equiv(\alpha,\beta)$,$\alpha,\beta\in R^N$,其中 L_ζ 是相空间中沿 ζ 方向平移的生成元,而 $\hat{L}_\zeta$ 是通过 Weyl 系统与 ζ 相联系的单参数群 $t\to W(t\zeta)$ 的生成元。

注意,(1)和(4)通过极限手续可以导出(2)和(3)。

在对应 $A\leftrightarrow\hat{A}$ 下,线性辛映射对应酉变换。但对非线性映射一般不成立。

可以证明,条件(1)~(5)给出映射 $A\leftrightarrow\hat{A}$ 的完全的刻画。而且,该对应不能扩展到相空间的其他函数上。确实,我们有

定理 3(van Hove) 令 G 表示 R^{2N} 上整体辛流的生成元构成的 C^∞ 函数类。对 $g\in G$,令 $\Phi_g(t)$ 为相应的群。不可能对每个 g 都存在对应 $g\leftrightarrow\hat{g}$,使得 $\hat{g}(x,p)=g(\hat{x},\hat{p})$,这里 $\hat{g}$ 是自伴的。

我们把 Weyl 量子化描述为 Schwartz 类 S 中的函数与一组有界算子之间的对应。Weyl 量子化可以扩展到更广泛的函数类上。用这种方法构造出来的算子称作 Fourier 积分算符。我们使用了记号 $\hat{\sigma}\equiv\sigma(D,x)$。

我们有如下有用的定理(Robert 1987):

定理 4 令 $l_1\cdots l_k$ 为 R^N 中满足 $\{l_il_k\}=0$ 的线性函数。令 P 为一多项式,且 $\sigma(\xi,x)\equiv P[l_1(\xi,x),l_k(\xi,x)]$。那么

(i) $\sigma(D,x)$ 将 S 映射到 $L^2(R^N)$(中算子)且为自伴的;

(ii)若 g 是连续的,那么 $g(\sigma)(D,x)=g(\sigma(D,x))$。

可以证明,$\sigma(D,x)$ 可以扩展为 $S'(X)\to S'(X)$ 的连续映射,且有

定理 5(Calderon-Vaillancourt) 若 $\sigma_0\equiv\sum_{|\alpha|+|\beta|\leqslant 2N+1}|D_\xi^\alpha D_x^\beta\sigma|<\infty$,算子 $\sigma(D,x)$ 的范数是以 σ_0 为界的。

通过 Weyl 量子化,从合适的函数类得到的算子称作伪微分算子。若 $\sigma(q,p)=P(p)$,其中 P 为一多项式,则 $\hat{\sigma}(p,q)$ 为微分算子。

另外,若 $\sigma(p,x)\in L^2$,那么 $\sigma(D,x)$ 是 Hilbert-Schmidt 算子,且

$$|\sigma(D,x)|_{HS}=(2\pi\hbar)^{-n/2}\left[\int|A(z)|^2\mathrm{d}z\right]^{1/2}$$

伪微分算子是非常重要的,特别是在分子的量子理论中(Le Bris 2003),那里绝热分析和 Peierls 替换规则迫使人们使用伪微分算子。

量子化理论中的下一个重要问题和动力学相关。

令 β 为一量子化过程,$H(p,q)$ 为相空间中一经典哈密顿量。令 A_t 为经典可观察量 A 在具有由 H 定义的流的时间演化,并假定 $\beta(A_t)$ 对所有 t 有很好的定义。

是否有自伴算符$\hat{H}$使得$\beta(A_t)=e^{it\hat{H}}\beta(A)e^{-it\hat{H}}$？如果有，是否可估计$|\hat{H}-\beta(H)|$？反过来，如果量子化流的生成元，按定义，是$\hat{H}$(像通常假定的那样)，那么是否可能对$\phi\in\mathcal{H}$的稠密集合估计出差$|(\beta(A_t)-(\beta(A))_t)\phi|$①，其中(对算子$\hat{A}$)$\hat{A}_t\equiv e^{it\hat{H}}\hat{A}e^{-it\hat{H}}$②？或者估计出差$|\tilde{A}_t-A_t|_\infty$，其中$\tilde{A}_t$定义为$\beta(\tilde{A}_t)=(\beta(A))_t$？对这些差，是否可能写成$\hbar$的渐近级数？

对于 Weyl 量子化，如果使用半经典可观察量，已经获得了一些定量结果(Robert 1987)。对于这点我们将不详细阐述。

为了更完备，我们简单介绍另一个量子化过程，它在数学物理中经常使用。

Wick 量子化

在这种量子化中，正函数对应正算符，但不保持多项式关系。它与 Bargmann-Fock-Segal 表示严格相关。

称以相空间中点(y,η)为中心的相干态为$(i\hat{p}+\hat{x}-i\eta+x)\phi_{y,\eta}(x)=0$的归一化解。

经典可观察量的 Wick 量子化是由映射$A\to Op^W(A)$定义的，其中

$$Op^W(A)\psi\equiv(2\pi\hbar)^{-n}\int A(y,\eta)(\psi,\bar{\phi}_{y,\eta})\phi_{y,\eta}dyd\eta$$

可以直接或通过 Weyl 表示证明，

(1) 若$A\geqslant 0$，则$Op^W(A)\geqslant 0$；

(2) 算子$Op_\hbar^W(A)$的 Weyl 符号是

$$(\pi\hbar)^{-n}\iint A(y,\eta)e^{\frac{1}{\hbar}[(x-y)^2+(\xi-\eta)^2]}dyd\eta;$$

(3) 对每个$A\in O(0)$有$\|Op_\hbar^W(A)-\hat{A}\|=O(\hbar)$。

Wick 量子化赋予每个矢量$\phi\in\mathcal{H}$一个相空间中的正 Radon 测度μ_ϕ，称作 Husimi 测度。它被定义为$\int Ad\mu_\phi=(Op_\hbar^W(A)\psi\cdot\psi)$，$A\in S(z)$。Wick 量子化不太适合处理非相对论粒子，特别是 Eherenfest 定理不能使用，且半经典传播定理的形式更加复杂。它常用于相对论量子场 Fock 空间中的分析，这时 Wick 排序扮演特别的角色。根据 Wick 排序，$\hat{x}_k$和$\hat{p}_k$的多项式要用产生湮灭算符重新排序：所有的产生算符都排在左边。

我们现在回到 Schrödinger 方程上来，注意它可以由哈密顿力学中N粒子系统的哈密顿量按照 Heisenberg 和 Weyl 量子化方案推导出来(至少在忽略自旋的情况下，因为自旋没有经典对应)。

除一些非本质的参量之外，R^3中N个标量粒子的 Schrödinger 方程可写成

$$i\hbar\frac{\partial\phi}{\partial t}=\sum_{k=1}^{N}(i\hbar\nabla_k+A_k)^2\phi+V\phi\equiv H\phi,\phi\in L^2(R^{3N}) \qquad [17]$$

其中A_k是R^3上的矢量函数(矢势)，$V=V_k(x_k)+V_{i,k}(x_i-x_k)$是$R^3$上的标量函数(标势)。

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① 原文误为$|\beta(A_t)-(\beta(A))_t|\phi$——译者注。

② 原文此处疑有笔误——译者注。

Schrödinger 量子力学中的典型问题如下:

(1)H 的自伴性,束缚态的存在性(算子的离散谱),它们的数目和分布,以及一般的谱性质。

(2)波算子

$$W_{\pm} \equiv s - \lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tH_0} \mathrm{e}^{-\mathrm{i}tH} \qquad [18]$$

的存在性,完备性和连续性,以及 S-矩阵与散射截面的确切存在性和性质。式[18]中 H_0 是合适的参考算子,通常为 $-\Delta$(并带有周期性边界条件,只要势在空间是周期性的),这时可以对 Schrödinger 方程或多或少做一些解析处理。

(3)半经典极限的存在性与性质。

在式[17]和式[18]中,我们隐含这样的假定:H 是不依赖时间的;当 H 依赖时间时会出现有趣的问题,特别是当它是时间的周期或准周期函数时,会有离子化现象。在周期性情形,Floquet 定理是有用的,但即便如此还是有很多有趣的问题没有解决。

如果势是充分规则的,H 的谱由一个绝对连续的部分(在空间是周期的情况下,由几个能带构成)和一个有少数聚点的离散部分组成。

另一方面,如果 $V(x,\omega)$ 在某些概率空间 Ω 中是可测函数,对(Ω 上)适当的分布(例如,高斯分布),谱几乎处处可能有完全不同的性质。例如,在 $N=1$(这时没有 $V_{i,j}$ 这种项),空间维数为 1 或 2 的情况下,谱是纯点且稠密的,本征函数在无穷远处指数衰减(尽管不是一致的);结果是演化群不会给出色散运动。同样的结论在三维也存在,如果势充分强且初态的动能充分受限。这种有趣的行为粗略地讲是由于势垒的随机性,且在很大程度上对空间准周期势也会出现(Pastur 和 Figotin 1992)。

和大量与 Schrödinger 方程相关的问题一样,算子 $(\boldsymbol{H}-\lambda\boldsymbol{I})^{-1}$ 在这里扮演着至关重要的角色,这里 λ 是一个在 $\boldsymbol{H}$ 的谱之外的复数;当 $(\boldsymbol{H}-\lambda\boldsymbol{I})^{-1}-(\boldsymbol{H}_0-\lambda\boldsymbol{I})^{-1}$ 是紧致算子时已经得到很多结果。

(1)型与(2)型问题在物理上很有趣,且与理论物理和量子化学有共同之处(Le Bris 2003),尽管研究手段与数学物理有些不同。半经典极限通常更有理论趣味,但它的分析与量子化学有关,并且在可以方便地使用多尺度方法时它非常有用,就像在分子谱的研究中那样。

我们从对(3)的简短描述开始;它提供了一种在物理常数 $\hbar$ 取很小值的单位制(在 CGS 单位制中 $\hbar \approx 10^{-27}$)中描述量子力学系统的有效的方法。从 Heisenberg 交换关系 $[\hat{x},\hat{p}] \subset \hbar\boldsymbol{I}$,可知位置和动量变量的色散(不确定度)的乘积正比于 $\hbar$,因而至少这两个量中的一个必须有非常大的值(与 $\hbar$ 相比)。通常考虑的情况是他们的色散大小相当,因而都非常小,量级为 $\hbar^{1/2}$(但与 $\hbar$ 相比很大)。为了和经典力学的 Hamilton-Jacobi 形式相联系,也可以考虑动量的色散是 $\hbar$ 量级的情况(WKB 方法)。

半经典极限在数学上的优势来源于自然单位制下参数 $\hbar$ 非常小的事实,因而可以进行渐进分析,这时"最低阶"可被准确描述且误差是可估计的。我们面对的问题是在"数学极限"$\hbar \to 0$ 下,Schrödinger 方程变成非常奇异的偏微分方程(微分项的系数趋向于零)。

将方程的每一项都除以 $\hbar$(因为我们不想改变时间标度),考虑 R^3 中有一个量子粒子位于势 $V(x)$ 中的情况(为简单起见,我们只考虑这种情况),得到

$$i\frac{\partial\phi(x,t)}{\partial t}=-\hbar\Delta\phi(x,t)+\hbar^{-1}V(x)\phi(x,t) \qquad [19]$$

因此,用因子 $\hbar^{1/2}$ 重新标度空间变量是方便的(即选另外的单位制),令 $x=\sqrt{\hbar}X$ 然后寻找式[19]的解,该解作为重新标度的变量 X 的函数在 $\hbar\to 0$ 时仍然是规则的。我们要在"物理尺度"上寻找解,使得它在该极限下可以"任意小"。所以,在该极限下这些解可以描述点粒子并不奇怪;半经典分析的主要结果是这些粒子的坐标服从经典力学的哈密顿法则。

这可以从如下的分析中粗略地看出来(为了使经验式的分析精确化,需要准确的估计)。用多尺度分析可以写出形如 $\phi(X,x,t)$ 的解,并寻找关于 X 和 x 是光滑的解。式[19]右边的两项都包含 $\sqrt{\hbar}$ 的 -2 或 2[①] 阶贡献,为了得到规则的解就必须让具有相同奇异性的贡献相互抵消掉。为了这一点,必须把势在某个适当的轨道 $q(t)$,$q\in R^3$ 附近展开到二阶(假定势至少是二次可微的),这条轨道要选得恰好使奇异性相互抵消。

形式分析表明,只有在轨道选得恰好是经典 Lagrange 方程的解时才能做到这一点。当然,为了使论据更加准确,更精细的分析和良好的估计是需要的,还需要估计出在导出的方程中忽略 $\sqrt{\hbar}$ 阶的项造成的误差;比较顺利的情况下,对每个给定的 T,在我们所描述的大多数类型的初始条件下,解的误差对于 $t<|T|$ 是 $\sqrt{\hbar}$ 量级。

这种半经典结果在 Wigner 函数框架下最容易看出来(优点是用于形式证明的技术细节可以采用函数论中的正则估计)。

在自然单位制下,我们定义

$$W_{\hbar,\rho}(x,\xi,t)=\left(\frac{i}{2\pi}\right)^N W_\rho\left(x,\frac{\xi}{\hbar},t\right)$$

用 Wigner 函数 $W_{\hbar,\rho}$,Schrödinger 方程[19]取如下形式

$$\frac{\partial f^\hbar}{\partial t}+\xi\cdot\nabla_x f^\hbar+K_\hbar * f^\hbar=0,\rho^\hbar(t=0)=\rho_0(\hbar) \qquad [20]$$

其中

$$K_\hbar=\frac{i}{(2\pi)^N}e^{-i\xi\cdot y_\hbar^{-1}}\left[V\left(x+\frac{\hbar y}{2}\right)-V\left(x-\frac{\hbar y}{2}\right)\right]$$

可以证明(Robert 1987),如果势充分规则且初始数据在适当的拓扑下收敛到一个正测度 f_0,那么对所有时间,$W_{\hbar,\rho}(x,t)$ 都会收敛到 Liuville 方程

$$\frac{\partial f}{\partial t}+\xi\cdot\nabla_x f-\nabla V(x)\cdot\nabla_\xi f=0$$

的一个(弱)解。如果,比如说考虑一系列初始数据 ρ_{ϕ_n},其中 ϕ_n 是一系列以 x_0 为中心而其 Fourier 变换以 p_0 为中心的函数,且其关于坐标和动量的色散都是 $\hbar^{1/2}$ 阶,上述结果导致半经典极限。这种情况下,极限测度是以经典路径为中心的 Dirac 测度。

在半经典极限定理的证明过程中,人们意识到最多是 $\hat{x}$ 和 $\hat{p}$ 的二次函数的哈密顿量的特殊地位。很容易验证对这些哈密顿量 $\hat{x}$ 和 $\hat{p}$ 的期待值服从经典的运动方程(P Ehrenfest 定则)。

从 Heisenberg 的观点看,这可以理解为下述事实的结论:对 a 和 a^* 至多是双线性的

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① 原文误为"-1" ——译者注。

算子在交换关系下构成代数 D,而且二阶齐次部分是一个闭的子代数,它对 D 的作用(通过交换)具有和哈密顿流及其切流的生成元代数一样的结构。除了(重要的)技术原因外,半经典极限定理的证明可以被简化为证明我们能估计出量子哈密顿量在经典轨迹上的展开式中高于二阶项的贡献在适当的拓扑下是 $\hbar^{1/2}$ 阶的(Hepp 1974)。

我们以一段对问题(1)和(2)的简短分析来结束本概述。(1)和(2)都是和那些直接可与实验数据相比较的现象有关的,因而在理论物理和量子化学中被广泛地研究(McWeeny 1992);其中一些现象已经采用数学物理的方法分析,且常常取得可观的成功。对这些问题我们这里只给出初等的介绍,希望读者通过阅读本百科全书中的专门条目去获得严格的分析和准确的陈述。

当然,大多数有物理兴趣的问题在如下意义下不是"精确可解"的,即最终结果很少能用简单函数明显地写出来。结果是,很少能获得相关物理问题的可与实验数据比较的精确数值结果,大多数情况下我们依赖对误差能做精确估计(如果顺利的话)的近似方案。

形式微扰论是这类方案中最简单的,但它很少给有物理兴趣的问题以可靠的结果。令

$$H_\epsilon \equiv H + \epsilon V \qquad [21]$$

其中 ϵ 为小的实参数,可如下给出情形(1)的一个形式方案

$$H_\epsilon \phi_\epsilon \equiv E_\epsilon \phi_\epsilon, E_\epsilon \equiv \sum_0^\infty \epsilon^k E_k, \phi_\epsilon \equiv \sum_0^\infty \epsilon^k \phi_k$$

和通过迭代 Duhamel 公式给出情形(2)的一个形式方案

$$\mathrm{e}^{-\mathrm{i}tH_\epsilon} = \mathrm{e}^{-\mathrm{i}tH①} + \mathrm{i}\epsilon \int_0^t \mathrm{e}^{-\mathrm{i}(t-s)H_\epsilon} V \mathrm{e}^{-\mathrm{i}sH_0 \mathrm{d}s} \qquad [22]$$

很少有情况使微扰级数收敛,人们必须求诸更精致的方法。

在某些情况,考虑 E_ϵ(作为 ϵ 的可微函数)的形式主部 $\tilde{E}_\epsilon$ 是方便的,并证明它在 $0<\epsilon<\epsilon_0$(不含 $\epsilon=0$)时对 ϵ 是可微的。在顺利的情况下,该方法可以导致

$$E_\epsilon = \sum_0^N \epsilon^k E_k + R_N(\epsilon), \lim_{\epsilon \to 0} |R_N(\epsilon)| = 0②$$

其中要有对 $0 \leqslant \epsilon < \epsilon_0$ 时 $|R_N(\epsilon)|$ 的明显估计。

某些情况下,形式幂级数的重求和技术可能有用。

一个下有界的算子的最低本征值通常可以用如下的变分法估计:对二次型 $Q(\phi) \equiv (\phi, H\phi)$ 应用最小最大技术。

半经典分析有助于寻找本征值的分布和研究那些在 $\hbar=1$ 单位制下坐标和动量色散都很大的态的动力学。

分子和原子物理中有一类特别有趣的情况,即如果出现在 H_ϵ 中的物理参数(典型量是过程中粒子的质量)能使我们先验地猜出有快速依赖时间的坐标存在(快变量)且这些坐标的补集对时间依赖很慢。这就建议我们可以尝试渐近分析,通常与绝热技术相联系。人们处理的情况很少有满足基本绝热定理的假设的,这时就必须改进分析,通常要通过微

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① 原文误为 H_0—— 译者注。

② 原文误为 $\lim_{N\to\infty} |R_N|(\epsilon) = +\infty$,与微挠论思想不符——译者注。

妙的估计来保证准不变子空间的存在性。

渐近技术和改进的估计在有效描述当 N 很大时由 N 个相互作用全同粒子组成的系统时也是需要的;例如在统计力学中,人们寻找在 $N\to\infty$ 时还成立的结果。

这个方向上最引人注目的结果是 E Lieb 及其合作者的关于物质稳定性的证明和 Bose-Einstein 凝聚现象及其相关的 Gross-Pitaevskii(非线性 Schrödinger)方程的研究。实验上发现对应于 Bose-Einstein 凝聚的物质态是即便在宏观尺度上物质的非经典行为的一个明确的证据。从数学物理的观点看,这个方向上正在进行的研究非常有挑战性。

我们也必须认识到,与应用和持续成功的纳米技术相关的量子力学研究变得越来越重要。从数学物理角度看,对纳米结构(限制在很小空间区域或低维流形,如面、线等——的量子力学系统)的研究还处于幼年,人们需要更精致的数学技术和全新的观念。

最后,必须强调数值分析(Le Bris 2003)特别是计算机模拟扮演的重要角色。对多粒子系统问题,当前的解析方法最多给出一些定性的估计,和在顺利的时候给出感兴趣的量的取值范围。近似方法并不总是有用的,并且经常是不可靠的。

与量子力学中我们感兴趣的物理现象(大多在凝聚态物理中)相关的数学处理的进展可能来源于用大型计算机上模拟的第一原理分析;这可能给出在典型初始条件下 Schrödinger 方程的解的定性,或在某种程度上的定量行为。如今,更有效的计算工具已经使计算机模拟更加可靠,更说明数学研究适合于对量子力学获得更全面的理解。

诠释问题

本节我们在量子力学框架内或用完全不同的方法讨论一些困扰当今量子力学的概念性问题,以及为解决这些问题而做的努力。

量子力学框架内的方法

我们从量子力学本身开始。我们已经指出测量问题的主要障碍是描述在测量的过程中到底发生了什么。公理 III 要求测量必须被看作一种"破坏"作用,测量结果在某种程度上是随机的。系统的末态是可观察量的本征态之一,对初态的依赖只是通过一个先验的概率分配;因此测量作用不具有因果性,这与系统与环境的相互作用的(连续)的因果可逆性描述不同。我们必须能先验地区分测量作用和一般的相互作用。

还有其他的困难。由于叠加原理,如果我们要在一个系统 S 中对算子 A 的性质做一次测量,S 就要和用算子 A 描述的测量工具 I"相互作用",组合系统的末态 ξ 将是这两个系统的(归一化)本征态的张量积的相干叠加

$$\xi=\sum_{n,m}c_{n,m}\phi_n^A\otimes\varphi_m^S,\ \sum_{n,m}|c_{n,m}|^2=1 \qquad [23]$$

量子力学的公理 III 所描述的测量要求,一旦测量过程结束,被测系统以几率 $\sum_m|c_{n,m}|^2$ 处在某个态 ϕ_n^A 上,而测量工具处在一个携带系统末态信息的态(毕竟,我们最后得到的是测量工具末态的读数)。

因此,将 ξ 写成如下形式:

$$\xi=\sum d_n\phi_n^A\otimes\zeta_n,\ \sum_n|d_n|^2=1 \qquad [24]$$

(当 A 的谱是纯点且不退化时,这定义了 ξ_n)。从式[24]看出,由于约化公设,我们知道,

如果对本征矢为$\{\zeta_n\}$,本征值为$\{z_n\}$之具有非退化谱的算子 T 进行一次测量,被测系统处于态 $\phi^A_{n_0}$,给出结果 z_{n_0}。

用这样的方法,我们没有解决测量问题(测量结果仍然是概率性的),但至少我们能找到理由说明为什么测量设备可以看作"经典的"。

回到式[23]来讨论是方便的。假定能够这样构造测量设备,它的纯(微观)态可以(大体上)分成一些集合 Φ_n(每个对应一个"宏观"态),Φ_n 与 A 的本征态(大体上)一一对应。集合 Φ_n 包含大量(N_{Φ_n})元素,所以集合 Φ_n 不需要极其精确地给定。并且集合 Φ_n 必须在小的外界扰动下是"稳定的"。

从这个粗略的描述中看得很清楚,测量设备应该包含大量的小组件,它们和"小"系统 A 的相互作用仍然会或多或少地导致集合 Φ_n 突然变化。

该机制的一个具体的模型由 K Hepp(1972)提出,他考虑 $\boldsymbol{A}$ 为一个 2×2 矩阵,测量设备是由 N 个自旋构成的链,$N\to\infty$;最近 Sewell(2005)完成了一个对有限但很大的 N 的含有误差估计的分析。这是一个动力学模型,其中可观察量 A(自旋)与自旋链相互作用("挪开自旋")后留下它经过的痕迹。正是这种痕迹(测量设备的末态宏观态)是可观察的且与 A 的末态相关。相互作用不是"瞬时的"而是需要很短的时间,具体依赖于描述设备和相互作用所用的参数。

我们称由于与环境的相互作用导致叠加原理的削弱为"退相干"。

有两个不同的退相干模型被详细地分析过了;我们将称它们为热浴模型和散射模型;两者都是动力学模型且在不同范围内都是约化问题的解,所谓约化问题是指约化到与算子 A 相交换的末态密度矩阵(因此导致干涉项的压低)。

热浴模型使用 Heisenberg 表象且依赖 C^* 代数理论的结果。这种方法与(量子)统计力学关系密切;它的目标是证明,在以热环境的自由度为条件下,被测系统的可交换算子集扮演特殊角色,它们是以概率形式给定测量结果的可观察量。

散射方法依赖于量子力学的 Schrödinger 方法和散射理论的结果。这种方法描述系统 S(典型情况是重粒子)与由大量轻粒子组成的环境的相互作用,然后试图在我们不知道任何轻粒子末态信息的情况下描述相互作用后 S 的态。人们试图去证明约化密度矩阵在一个给定的表象(典型情况是由空间坐标确定的)中(几乎)是对角的。这就定义了可以测量的观察量(典型情况为位置)以及每次结果的概率。

这两种方法都是依靠测量过程中信息的丢失来抵消叠加原理的效应,将测量问题带入经典概率论的框架中。它们都无法提供测量结果对系统初态的因果依赖性。

我们对这些尝试只做很简单的描述。

在更基础的形式上,"散射方法"的出发点是两粒子系统的 Schrödinger 方程,其中一个粒子的质量远比另一个小。重粒子可以看作我们要测量的系统。主要的分析方法(如果顺利的话可以严格处理)如下(Joos 和 Zeh 1985, Tegmark 1993)。选取单位制使重粒子质量为 1,轻粒子质量为 ϵ。如果 x 是重粒子的坐标,y 是轻粒子的坐标,系统的初态是 $\Phi_0(x,y)$,则系统的方程的解就是(除去不重要的因子)

$$\Phi_t = \exp\{i(-\Delta_x - \epsilon^{-1}\Delta_y + W(x) + V(x-y))t\}\Phi_0$$

使用质心系和相对坐标,可看出当 ϵ 非常小时可以在两个时间尺度上描述该系统,一个快(轻粒子)尺度和一个慢(重粒子)尺度,因而我们可以使用绝热技术。在该框架中,对重粒

子的测量(例如,它的坐标)可以通过考虑处于散射区域的轻粒子,然后使用对应于势 $V_x(y)\equiv V(y-x)$ 的波算符。

对轻粒子自由度求部分迹(对应没有末态信息),我们发现,至少具有启发性,现在重粒子的态可用密度矩阵 $\boldsymbol{\sigma}$ 描述(由于迹运算)。$\boldsymbol{\sigma}$ 在坐标表象中的非对角元 $\sigma_{x,x'}$ 被因子 $\xi_{x,x'}=1-(W_x^+\psi,W_{x'}^+\psi)$ 略微压低,其中 ψ 表示轻粒子的初态,W_x^+ 是轻粒子在势 ϵV_x 中运动的波算符。必须假设表示重粒子初态的函数 ϕ 是充分定域化的以致对 $x'\neq x$ 有 $\xi_{x,x'}<1$。

如果环境是由大量粒子组成(它们的数目 $N(\epsilon)$ 必须满足 $\lim_{\epsilon\to 0}N(\epsilon)=\infty$),假设重粒子可以和所有粒子分别作用,那么当 $\epsilon\to 0$ 时,密度矩阵的非对角元趋向于 0,最后密度矩阵趋向于形式 $\Phi(x,x')=\delta(x-x')\rho(x)$,$\rho(x)\geqslant 0$,$\int\rho(x)\mathrm{d}x=1$。如果可以假设所有相互作用在时间 $T(\epsilon)\leqslant\epsilon^{\alpha}(\alpha>0)$ 发生,则有 $\rho(x)=|\psi(x)|^2$。

如果相互作用不是独立的,分析会变得棘手得多,因为必须用多体散射理论来处理;这意味着散射方法很难用到"热浴模型"中。在任何情况下,选择一组"优先基"(坐标表象)依赖于处理的是散射现象这一事实。严格的分析也有一些进展(Teta 2004),但我们离数学上满意的答案还很远。

热浴方法已经在量子力学的代数框架中研究过,其数学基础比较好(Alicki 2002, Blanchard et al. 2003, Sewell 2005)。它的缺点是很难把形式方案和实际物理情形联系起来,也很难给出退相干时间的实际估计。

热浴方法把退相干效应归因于实际上不可能区分系统大量的纯态和相应的统计混合。在这种方法中,可观察量被表示为 Hilbert 空间 $\mathcal{H}$ 上所有有界算子 $\mathcal{B}(\mathcal{H})$ 的弱闭子代数 $\mathcal{M}$ 中的自伴元。该子代数可能依赖于测量设备(即不是所有的设备都适合于测量一组可观察量)。"经典"可观察量,按定义,与所有其他的可观察量交换,因此必须属于 A 的中心,该中心与某概率空间 $\mathcal{M}$ 上的一组函数同构。所以量子系统中经典性质的出现对应具有非平凡中心的代数的"出现"。因为代数的自同构演化是保持中心不变的,这个过程只有在允许丢失量子相干性的情况下才能实现;这就要求我们描述的量子系统是开的并与环境相互作用,而且出现的交换代数随时间演化将是稳定的。

可以证明必须要考虑热力学极限下的量子环境,即考虑被测系统与热环境的相互作用。Gellmann(1993)曾讨论过经典可观察量的可能出现和相应的动力学。在所有这些方法中,交换子代数都是由相互作用的特殊形式选定的;因此,测量设备决定了经典可观察量的代数。

在实验方面,使用非常精巧的技术已经获得了大量有趣的结果;这些实验通常也确定了"退相干时间"。无论对碰撞模型(Hornberger et al. 2003)还是热浴模型(Hackermueller et al. 2004)的实验结果,大都是用富勒烯(一种很重的分子,被气体中的粒子碰撞后不会偏转得太多)完成的。它们与(粗糙的)理论结果符合得较好。

关于退相干的最精巧的实验是那些与量子光学有关的实验(超导容器中的圆偏振原子)。它们与粒子束的波动性无关,而是与单光子的"波本质"有关。电磁场现在被看作任意大数量的光子态的非相干叠加。偏振光子能一个一个地产生,它们保持独立性和偏振直到它们每个都与"环境"(例如,容器的边界或气体中的粒子)发生相互作用。在某种意

义下,这些实验结果对应于"碰撞退相干"理论。

Haroche(2003)的实验证明相干性可以持续一段可观测的时间,这是至今关于相干性控制的最好的实验。

其他方法

我们通过关于"隐变量"问题的简要讨论来介绍一种关于量子力学的完全不同的处理方法来结束本节,它们是 D Bohm(1952)首创的,最近被 Duerr 等人(1999)建立在牢靠的数学基础上。这种方法从根本上不同于传统的量子力学,现在还不清楚它是否能解决测量问题并且描述那些传统量子力学能处理的所有现象。但从数学的角度看它是非常有趣的。

我们已经评论过量子力学的表述——概括在早先给出的 3 个公理中——有很多令人不满意的地方,主要是与叠加原理(在极端情况下可以用 Schrödinger 猫佯谬描述)和测量问题相关的那部分,后者显示出,例如通过 Einstein-Rosen-Podolski 佯谬,量子力学的内在非定域性,即对距离很远的系统依然可以保持它们的"客观"性。从量子力学建立之初,就一直有很多尝试把这些特性归因于存在"隐变量";从这种观点看,量子力学预言的统计本质是由于描述系统的参数的不完备性。量子力学的统计预言(由实验发现所确认)与基于隐变量和经典概率论的定域理论之间的不可匹配性已为人们所知(Kochen 和 Specher 1967),这也可通过"Bell 不等式"(Bell 1964)知道,其中 Bell 不等式关于纠缠系统(主要是产生于适当纠缠态中的两光子或两自旋 1/2 的粒子)的分别测量结果的关联间的不等式。

关于量子力学的内在非定域性(在如上所述的意义下)的证明由 L Hardy 给出(见 Haroche 2003)。

尽管实验结果证明,不能简单地用隐变量理论来代替量子力学,但更巧妙一些的努力可能会成功。我们只讨论 Bohm 的方法(沿袭 de Broglie 的尝试),就像 Duerr 等人(1999)做的那样。这是一个动力学理论,用"经典路径"表征点,而时间依赖的矢量"速度"场支配着运动(在这种意义下,它是非牛顿的)。在某种意义下,如果保持坐标作为原始观察量,Bohm 力学是量子力学的最小实现。对这些原始量,Bohm 理论中加入一个定义在粒子构形空间 $\mathcal{Q}$ 中的复函数 ϕ(用 Bohm 的术语称作"导波")。当粒子有自旋时,ϕ 是一个旋量函数。动力学由两个方程给出:一个是关于粒子坐标的,一个是关于导波的。如果用 $x \equiv x_1, \cdots, x_N$ 描述点的构形,那么在势场 $V(x)$ 中的动力学就如下描述:波 ϕ 满足带势 V 的非相对论 Schrödinger 方程,坐标满足常微分方程

$$\dot{x}_k = (\hbar/m_k)\mathrm{Im}\left[\frac{\phi^* \nabla_k \phi}{\phi^* \phi}\right](x), x_k \in R^3$$

式中,m_k 是第 m 个粒子的质量。

注意,矢量场在波函数的零点是奇异的,因此整体存在性和惟一性必须证明。为了看出为什么 Bohm 力学在经验论上是等价与量子力学的,至少对坐标的测量是这样,我们注意到点的方程与量子力学的连续方程是一致的。这说明如果在时间为零时有一系列点按照密度 $|\phi_0|^2$ 分布,那么在时间 t 就按照密度 $|\phi(t)|^2$ 分布,其中 $\phi(t)$ 是 Schrodinger 方程在初值 ϕ_0 下的解。

Bohm(1952)通过引入一个"量子势"V_Q 将该理论表述为对牛顿定律的修改(这种表

述被广泛使用)。这可以通过把波函数写成极坐标形式 $\phi = Re^{iS/\hbar}$ 和把连续方程写成修改后的 Hamilton-Jocobi 方程做到。Bohm 理论的 Duerr 等人的(1999)版本只引入了导波函数和点的坐标,且把理论建立在可靠的数学基础上。通过一系列令人印象深刻的数学结果,这些作者和他们的合作者处理了速度矢量场的完备性和点的轨迹的渐近行为(对散射区域和对束缚轨迹,表明它们对应量子力学的束缚态),为此他们严格分析了穿过曲面的通量定理(散射理论的基石),并通过研究与测量设备的相互作用仔细分析了双缝实验。该理论是完全因果性的,无论是对点的轨迹还是对导波的时间演化,且也可以适用于有自旋的点的情况。它导致对半经典极限的精确数学表述,它也可能解决测量问题,方法是把整个系统的导波和与被测粒子相关的导波的非相干叠加的近似分解联系起来,并和测量设备联系起来(这可能是看到量子力学中"波函数塌缩"的方法)。这种方法的弱点是表示点与可观察量之间的关系。

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导论:拓扑学

引言

本文是一篇关于一般拓扑学(general topology)的导论。我们将不会涉及代数拓扑学,尽管它在某些数学系里作为本科生的高级课程中被引入。代数拓扑学这一专题将会在本书关于上同调理论(Cohomology theories)的部分中得到处理。

我们相信这样一篇基础性的文章对于这部百科全书的用处纯粹在于为了快速的查阅。物理学家对于这里的绝大部分概念是熟悉的,但通常是在相当不精确的意义下。本文将提供严格的定义和结果,它们在参阅本书的其他文章时将被用到。为了保证确实如此,我们实际上在物理学家那里检测了本文的实用性。

拓扑学经常被描述成"橡皮膜上的几何学"(rubber-sheet geometry),也就是说,人们可以在不撕裂的情况下形变所研究的对象。这是关于连续性的最重要的概念。连续性是我们在这里所要研究的绝大部分问题的基础。

我们将给出完整的定义,严格地陈述定理,但不会给出任何证明的细节。另一方面,从应用于数学物理的角度出发,在假定对于未加定义的更高级的概念熟悉的情况下,我们将引用大量的例子。论题的选择也是基于同样的理由。

基本概念

定义 1 设 X 为一集合。X 的一族子集 $\mathcal{T}$ 称为一个拓扑(topology),如果以下性质成立:

(i) $\phi, X \in \mathcal{T}$

(ii) 令 $\mathcal{I}$ 为一指标集,则

$$A_\alpha \in \mathcal{T}, \alpha \in \mathcal{I} \Rightarrow U_{\alpha \in \mathcal{I}} A_\alpha \in \mathcal{T}$$

(iii) $A_i \in \mathcal{T}, i = 1, \cdots, n \Rightarrow \bigcap_{i=1}^{n} A_i \in \mathcal{T}$

定义 2 拓扑 $\mathcal{T}$ 中的一个成员称为(X 在拓扑 $\mathcal{T}$ 下的)一个开集(open set)。

评注 最后两条性质可以更容易地表述为开集的任意并是开集,开集的有限交是开集。这一点的重要性是显而易见的:如果我们在实直线(real line)上取"通常的拓扑"(usual topology)(其定义在下文中给出),则所有开区间$(-1/n, 1/n)$(n 是一个正整数)的交集是一点$\{0\}$,在一般意义下显然不是开的。

例子 如果假定 ϕ 和 X 是仅有的开子集,则得到所谓的非离散拓扑(indiscrete topology) 或最粗拓扑(coarsest topology)。另一个极端情形是假定所有的子集都是开集,则我们得到离散拓扑(discrete topology)或最细拓扑(finest topology)。如果我们以实直线或平面为例来考虑,这两个拓扑都不太自然。但事实上如果我们从定义中明确地排除它们则会更不自然。在某些方面它们显得非常有用。

定义 3 X 的一个子集称为闭的(closed),如果它在 X 中的余集是开的。

评注

(i)基于并集的补集等于补集的交集这一简单的关系,我们可以很容易地用闭集代替开集来构造一个拓扑。

(ii)从定义来看,没有什么理由排除一个集合可能是既开又闭,或非开非闭的。否定这种可能是一个常见的错误。

定义 4 一个被赋予了拓扑的集合称为一个(关于给定拓扑的)拓扑空间(topological space)。拓扑空间中的元素有时被称为点。

定义 5 令 $x \in X$。x 的一个邻域(neighbourhood)是 X 的一个子集,该子集包含一个含有 x 的开集。

评注 这个定义看起来有些不方便,但实际上在一般情况下比通常那种仅限于开邻域的定义要有用。

定义 6 一个开集的子族 $\mathcal{B} \subseteq \mathcal{T}$ 称作拓扑 $\mathcal{T}$ 的一个基(*basis*),如果每个开集都是 $\mathcal{B}$ 中集合的并集。

定义 7 一个开集的子族 $\mathcal{S} \subseteq \mathcal{T}$ 称作拓扑 $\mathcal{T}$ 的一个子基(*sub-basis*),如果每个开集都是 $\mathcal{S}$ 中集合的有限交集的并集。

定义 8 X 的子集 A 的闭包(closure) $\bar{A}$ 是(X 中)包含 A 的最小闭集。

定义 9 X 的子集 A 的内点(interior)$\mathring{A}$ 是(X 中)包含于 A 的最大开集。

评注 有时定义集合 $\bar{A}/\mathring{A}=\{x \in \bar{A}, x \notin \mathring{A}\}$ 为 A 的边界(boundary)。

定义 10 设 A 为拓扑空间 X 的子集。点 $x \in X$ 称为 A 的极限点(limit point),如果每一个包含 x 的开集都包含 A 中异于 x 的点。

定义 11 称 X 的子集 A 在 X 中稠密(dense),如果 $\bar{A}=X$。

定义 12 拓扑空间 X 称为 Hausdorff 空间(Hausdorff space),如果对于任意不同的两点 $x, y \in X$,存在 x 的开邻域 A 与 y 的开邻域 B,使得 A 与 B 不相交(即 $A \cap B=\phi$)。

评注与例子

(i)这看起来更像我们所期待的。但是,某些略微非 Hausdorff 的空间会很有用。例如,在 twistor 理论中。一个"口袋"(pocket)提供了这样的一个例子。考虑实平面的子集 X,由实轴上的区间 $[-1,1]$ 和直线 $y=1$ 上的区间 $[0,1]$ 构成,并且等同如下的点:$(x,0) \approx (x,1), 0<x \leqslant 1$。这样,点 $(0,0)$ 与 $(0,1)$ 就没有不相交的开邻域。严格说来,我们将需要下文中引入的商拓扑的概念。

(ii)一个更加"地道"的非 Hausdorff 空间:考虑正整数组成的空间 $\mathbf{N}=\{1,2,3,\cdots\}$,开集取成 $\phi, \mathbf{N}$ 以及集合 $\{1,2,3,\cdots,n\}$,对每一个 $n \in \mathbf{N}$。这个空间既非 Hausdorff 亦非紧致(见后面关于紧致的定义)。

定义 13 设 X, Y 为拓扑空间,$f: X \to Y$ 为一个从 X 到 Y 的映射。我们称 f 是连续的(continuous),如果对于 Y 中任意开集 A,$f^{-1}(A)$ 是 X 中的开集。

评注 连续性是这里最为重要的概念。在这个一般的框架下,它看起来与"$\varepsilon-\delta$"定义略有不同。但是后者只对于度量空间有效。我们马上将要谈到度量空间。

定义 14 一个映射 $f: X \to Y$ 称作同胚(homeomorphism),如果它是连续的双射,并且它的逆映射 f^{-1} 也是连续的。

评注 两个同胚的空间从拓扑学的观点来看是不可区分的。在这个意义下,同胚是拓扑空间之间自然的映射。拓扑不变量就是拓扑空间在同胚下保持不变的性质。

定义 15 设 $B\subseteq A$。我们可以定义 B 的相对拓扑(relative topology):一个子集 $C\subseteq B$ 是开集当且仅当存在 A 的开集 D 使得 $C=D\cap B$。

定义 16 一个赋予了相对拓扑的子集 $B\subseteq A$ 称为拓扑空间 A 的子空间。

评注 这样,对于实直线的子集,如果我们令 $A=[0,3]$,$B=[0,2]$,则在由 $\mathbf{R}$ 上通常拓扑诱导的相对拓扑下,$C=(1,2]$是 B 中的开集。

定义 17 给定两个拓扑空间 X,Y,我们可以定义乘积拓扑空间(product topological space) $Z=X\times Y$。这里 Z 作为集合是 X 和 Y 的笛卡儿积。令 A 为 X 中开集,B 为 Y 中开集,则形如 $A\times B$ 的集合构成 Z 的一个拓扑基。

评注 注意 $X\times Y$ 中的开集并不一定都具有乘积$(A\times B)$的形式。

定义 18 设对于指标集 $\mathcal{I}$,有一个将 X 分成互不相交的子集 A_α,$\alpha\in\mathcal{I}$,的分解。或者等价地说,在 X 上定义了一个等价关系$\sim$。则我们可以按以下方式在等价类的集合 $\{A_\alpha,\alpha\in\mathcal{I}\}$,(通常记作商空间(*quotient space*) $X/\sim=Y$)上定义商拓扑(quotient topology)。考虑正则投影映射 $\pi:X\to Y$,它把 X 中的一个元素 x 映到它的等价类$[x]$。则 Y 中的子集 $U\subseteq Y$ 是开集当且仅当 $\pi^{-1}(U)$是开集。

命题 1 令 $\mathcal{T}$为商空间 Y 上的商拓扑。设 $\mathcal{T}'$为 Y 上另一个拓扑使得正则投影是连续映射,则 $\mathcal{T}'\subseteq\mathcal{T}$。

定义 19 X 的一个(开)覆盖(open cover) $\{U_\alpha:\alpha\in\mathcal{I}\}$是指 X 的一族开子集 $U_\alpha\subseteq X$,它们的并集是 X。一个覆盖的子覆盖是指这族集合的一个子族,它本身也是 X 的一个覆盖。

定义 20 一个拓扑空间 X 称为紧致的(compact),如果 X 的每个覆盖都有有限的子覆盖。

评注 对于紧致空间来说,无论我们选择怎样的覆盖,用有限个开子集就足够了。这是开区间(非紧致)和闭区间(紧致)的根本区别。前者实际上同胚于整个实直线。

定义 21 一个拓扑空间 X 称为连通的(connected),如果它不能写成两个互不相交的非空开集的并。

评注 一个有用的等价定义是:任何一个从 X 到赋予离散拓扑的两点集合$\{0,1\}$的连续映射都不是满射。

定义 22 给定拓扑空间 X 中的两点 x 和 y,一条从 x 到 y 的路径(path)是一个连续映射 $f:[0,1]\to X$,使得 $f(0)=x$,$f(1)=y$。我们也称这条路径连接 x 和 y。

定义 23 一个拓扑空间 X 称为路径连通的(path-connected),如果 X 中的任意两点都可以被一条完全在 X 中的路径连接。

命题 2 路径连通的空间是连通的。

命题 3 $\mathbf{R}^n$ 中的连通开子空间是路径连通的。

定义 24 给定一拓扑空间 X,定义一等价关系如下:$x\sim y$ 当且仅当 x 和 y 属于 X 的同一个连通子空间。则每个等价类称为 X 的一个(连通)分支(connected component)。

例子

(i) 3×3 正交矩阵构成的李群 $O(3)$具有两个连通分支。单位连通分支是子群 $SO(3)$。

(ii) 闵可夫斯基时空(Minkowski space)中的洛伦兹变换(Lorentz transformation)构成洛伦兹变换群的单位连通分支。

度量空间

度量空间是一类具有重要地位的特殊的拓扑空间。

定义 25 一个度量空间(metric space)是一个集合 X 以及一个函数 $d:X\times X\to\mathbf{R}$,满足

(i)$d(x,y)\geqslant 0$

(ii)$d(x,y)=0\Leftrightarrow x=y$

(iii)$d(x,z)\leqslant d(x,y)+d(y,z)$ ("三角不等式"(triangle inequality))

评注

(i)函数 d 称作两点间的度量函数或距离函数。

(ii)在数学物理中度量的概念一般被理解为"欧氏度量"(Euclidean metric)。显著的特征是正定性(以及三角不等式)。我们可以,也确实会,引入具有不同符号的不定度量(例如闵可夫斯基度量)。但是这些度量不被用来在所关心的空间上诱导出拓扑。

定义 26 给定度量空间 X 中一点 $x\in X$,我们定义以 x 为中心 r(r 是一个正实数)为半径的开球(open ball)为

$$B_r(x)=\{y\in X:d(x,y)<r\}$$

给定度量空间 X,通过取 X 中所有开球为拓扑基,我们可以马上在 X 上定义一个拓扑。我们称这是由给定度量诱导的拓扑。于是我们可以重新得到关于连续性的通常的"$\varepsilon-\delta$"定义。

命题 4 令 $f:X\to Y$ 为度量空间 X 到度量空间 Y 的映射。则 f 在 $x\in X$ 处连续(对于所诱导的拓扑)当且仅当对任意 $\varepsilon>0$,存在 $\delta>0$,使得若 $d(x,x')<\delta$,则有 $d(f(x),f(x'))<\varepsilon$。

注意在这里我们并没给两个度量不同的记号,因为它们分别涉及哪个空间是很明显。通过取相关的球作为邻域,证明可以容易得到。同样容易得到如下命题:

命题 5 度量空间是 Hausdorff 的。

定义 27 一个度量空间之间的映射 $f:X\to Y$ 是一致连续的(uniformly continuous),如果对任意 $\varepsilon>0$,存在 $\delta>0$,使得对于所有 $x_1,x_2\in X$,若 $d(x_1,x_2)<\delta$,则有 $d(f(x_1),f(x_2))<\varepsilon$。

评注 注意连续和一致连续的差别:后者要更强而且对整个空间要求一致的 δ。

定义 28 在 X 上定义的两个度量 d_1 和 d_2 是等价(equivalent)的,如果存在正常数 a 和 b,使得对任意两点 $x,y\in X$,有

$$a\,d_1(x,y)\leqslant d_2(x,y)\leqslant b\,d_1(x,y)$$

评注 这显然是一个等价关系。两个等价的度量诱导出相同的拓扑。

例子

(i)给定集合 X,我们定义离散度量如下:$d_0(x,y)=1$ 若 $x\neq y$。它在 X 上诱导出离散拓扑。这是一个十分方便的描述离散拓扑的方法。

(ii)在 $\mathbf{R}$ 上,通常度量是 $d(x,y)=|x-y|$,$\mathbf{R}$ 上的通常拓扑由这个度量所诱导。

(iii)更一般地,在 $\mathbf{R}^n$ 上,对于每个 $p \geqslant 1$,我们可以定义一个度量

$$d_p(x,y) = \left\{ \sum_{k=1}^{n} |x_k - y_k|^p \right\}^{1/p}$$

这里 $x=(x_1,x_2,\cdots,x_n)$,$y=(y_1,y_2,\cdots,y_n)$。特别地,对于 $p=2$,我们得到欧氏度量,但是其他情形也是有用的。继续这个序列,可以定义

$$d_\infty = \max_{1 \leqslant k \leqslant n} \{ |x_k - y_k| \}$$

所有这些度量都在 $\mathbf{R}^n$ 上诱导出相同的拓扑。

(iv)在一个实数或复数域上的向量空间 V 上,一个函数 $\|\cdot\| : V \to \mathbf{R}^+$ 称为一个范数(norm),如果它满足以下公理:

(a) $\|x\| = 0$ 当且仅当 $x=0$,

(b) $\|\alpha x\| = |\alpha| \, \|x\|$,

(c) $\|x + y\| \leqslant \|x\| + \|y\|$。

易见利用范数可以定义一个度量

$$d(x,y) = \|x - y\|$$

在许多情况下,例如对于上面例子(iii)中定义的度量,我们可以把一个向量的范数定义成它到原点的距离。一个显然的例外是离散度量。

一个对于函数和算子空间很有用的,稍为一般的概念是半范数。一个半范数(seminorm)满足上面关于范数的公理中的后两条,但不一定满足第一条。

定义 29　给定一个度量空间 X,一个点列 $\{x_1,x_2,\cdots\}$ 称为柯西列(Cauchy sequence),如果对任意 $\varepsilon > 0$,存在一个正整数 N,使得对任意 $k,l > N$,有 $d(x_k,x_l) < \varepsilon$。

定义 30　在度量空间 X 中给定一个点列 $\{x_1,x_2,\cdots\}$,一点 $x \in X$ 称为这个序列的极限(limit),如果对任意 $\varepsilon > 0$,存在一个正整数 N,使得对任意 $n > N$,有 $d(x,x_n) < \varepsilon$。我们称这个序列收敛(converge) 到 x。

定义 31　一个度量空间 X 称为完备的(complete),如果它中的每个柯西列都在 X 中有极限。

例子

(i)实直线上的闭区间 $[0,1]$ 是完备的,而开区间 $(0,1)$ 则不是。例如,柯西列 $\{1/n, n=2,3,\cdots\}$ 在这个开区间上没有极限点(看成实直线上的序列,它当然有极限点 0)。

(ii)空间 $\mathbf{R}^n$ 实完备的。

(iii)由所有使得求和 $\sum_1^\infty x_k^2$ 收敛的实数序列 $\{x_1,x_2,\cdots\}$ 构成的希尔伯特空间(Hilbert space) l^2 它在前面定义的 d_2 的无穷维推广而得的度量下是完备的。对任意 $p \geqslant 1$,可以类似地定义 l^p,它们也是完备的,从而是巴拿赫空间(Banach space)。

评注　完备性不是拓扑不变量。例如,开区间 $(0,1)$ 与整个实直线同胚(在通常拓扑下),但是前者不完备而后者完备。同胚可以方便地由正切函数给出。

定义 32　度量空间 X 的一个子集 B 称为有界的,如果存在一个半径为 $R(R > 0)$ 的球,完全包含 B。

定理 1(Heine-Borel)　$\mathbf{R}^n$ 的任何有界闭子集是紧致集。

评注　逆命题亦成立。从而我们有一个非常好的关于 $\mathbf{R}^n$ 的紧致子集的刻画:有界

闭集。

命题 6 $\mathbf{R}^n$ 中的任何有界序列有一个收敛子序列。

定义 33 考虑定义在 $\mathbf{R}$ 的子集 A(通常为一区间)上的一列实值函数$\{f_n\}$。我们说$\{f_n\}$在 A 上逐点收敛(converge pointwise),如果对于每个 $x\in X$,实数列$\{f_n(x)\}$收敛。从而我们可以定义函数 $f:A\to\mathbf{R}$,$f(x)=\lim\limits_{n\to\infty}f_n(x)$,并记成 $f_n\to f$。

定义 34 一列函数 $f_n:A\to\mathbf{R}$,$A\subseteq\mathbf{R}$,称为一致收敛(converge uniformly)到函数 $f:A\to\mathbf{R}$,如果对任意 $\varepsilon>0$,存在一个正整数 N,使得对所有 $x\in X$,只要 $n>N$,就有 $|f_n(x)-f(x)|<\varepsilon$。

定理 2 令 $f_n:(a,b)\to\mathbf{R}$ 为一列函数,在 $c\in(a,b)$ 处连续。假设 f_n在(a,b)上一致收敛到 f,则 f 在 c 处连续。

注记和例子 连续函数的逐点极限不一定连续,这从以下例子中可以看出。令 $f_n(x)=x^n$,$x\in[0,1]$。我们看到极限函数 f 不连续。

定义 35 设 X 为一度量空间。一个映射 $f:X\to X$ 称为压缩映射(contraction),如果存在 $c<1$,使得对所有 $x,y\in X$,有 $d(f(x),f(y))\leqslant c\,d(x,y)$。

定理 3(Banach) 若 X 为一完备度量空间,f 为 X 上一压缩映射,则 f 在 X 上有惟一不动点 x,即 $f(x)=x$。

一些函数与算子空间

函数和算子空间上可以赋予不同的拓扑,它们由不同的收敛和范数(或半范数)的概念给出。通常对于同一个空间就有这些不同的概念。如前所述,向量空间上的一个范数给出一个度量,从而给出一个拓扑。类似地,利用函数和算子序列的收敛性的概念,我们可以知道什么是极限点,从而知道什么是闭集。

但是在这之前,让我们先在一个稍微不同的情形下引入一个拓扑。这个拓扑在某种意义下是空间之间连续映射所构成的空间上的自然拓扑。

定义 36 考虑从拓扑空间 X 到拓扑空间 Y 的一族连续映射 F,并定义 $W(K,U)=\{f:f\in F,f(K)\subseteq U\}$。则由所有具有形式 $W(K,U)$的集合构成的族构成 F 上的紧致开拓扑(compact open topology)的一个子基。这里 K 是 X 中紧致集,U 是 Y 中开集。

考虑拓扑空间 X 和其上的一列函数(f_n)。令 $D\subseteq X$。就像对于实直线的子集上的函数那样,我们可以定义逐点收敛和一致收敛。

定义 37 设 $X,D,(f_n)$如上,

(i)函数 f_n在 D 上逐点收敛(converge pointwise)到 f,如果对于任意 $x\in D$,数列 $f_n(x)$ 收敛,$f_n(x)\to f(x)$。

(ii)函数 f_n在 D 上一致收敛(converge uniformly)到 f,如果对任意 $\varepsilon>0$,存在一个正整数 N,使得对所有 $x\in D$,$n>N$,有$|f_n(x)-f(x)|<\varepsilon$。

下面我们考虑勒贝格空间(Lebesgue space) L^p,即定义在 $\mathbf{R}^n$ 的子集上,$|f(x)|^p$勒贝格可积的函数 f。这里实数 $p\geqslant 1$。在定义这些空间时,我们隐含地使用了几乎处处(即相差一个零测集)相等的函数的等价类。但通常我们总可以取这些等价类的代表元,从而和真正的函数打交道。注意对所有的 L^p,只有 L^2是希尔伯特空间。

定义 38 在空间 L^p 上定义范数

$$\| f \| = \left(\int | f(x) |^{p} \mathrm{d}x \right)^{1/p}$$

现在我们转到一般的赋范空间及其上的算子。

定义 39 按范数收敛也称为强收敛。换而言之,赋范空间 X 中的序列(x_n) 称为强收敛(converge strongly)到 x,如果

$$\lim_{n \to \infty} \| x_n - x \| = 0$$

定义 40 赋范空间 X 中的序列(x_n) 称为弱收敛(converge weakly)到 x,如果对所有有界线性泛函 f,有

$$\lim_{n \to \infty} f(x_n) = f(x)$$

考虑从 X 到 Y 的有界线性算子空间 $B(X,Y)$。通过定义如下范数我们可以使之成为一赋范空间。

$$\| T \| = \sup_{x \in X, \| x \| = 1} \| Tx \|$$

于是我们可以在 $B(X,Y)$上定义 3 种不同的收敛性。实际上,在当前的泛函分析中还有更多的收敛性。

定义 41 设 X,Y 为赋范空间,(T_n)为一列算子,$T_n \in B(X,Y)$ 。

(i)(T_n)一致收敛(uniformly convergent),如果它按范数收敛。

(ii)(T_n)强收敛(strongly convergent),如果对任意 $x \in X$,$(T_n x)$ 强收敛。

(iii)(T_n)弱收敛(wealy convergent),如果对任意 $x \in X$,$(T_n x)$ 弱收敛。

注记 显然有一致收敛⇒强收敛⇒弱收敛,并且在这 3 种情况下极限相同。但反过来通常不成立。

同伦群

拓扑空间 X 最基本和明显的性质是它的连通分支的个数。下一个这样的性质,在某种意义上,是 X 中洞的个数。存在更高阶的类似物,称为同伦群(homotopy groups)。它们是拓扑不变量,即在同胚下保持不变。它们在场论和其他数学物理问题的拓扑考虑中具有重要的地位。文章 Topological Defects and Their Homotopy Classification 和 Electric-Magnetic Duality 含有一些这样的例子。

定义 42 给定拓扑空间 X,它的第 0 个同伦集(homotopy set)是它的连通分支的集合,记做 $\pi_0(X)$。当 X 是连通的时,有时记做 $\pi_0(X)=0$。

为了定义 X 的基本群,或 $\pi_1(X)$,我们需要环路的概念。它在其他方面也是有用的。为简单起见,我们将考虑带基点的环路(即通过 X 上一个固定点的环路)。在绝大部分的应用中,它们是相关的对象。我们可以考虑具有各种不同光滑性的环路(当 X 是一流形时),但从量子场论应用的角度来看,我们将考虑连续的环路。它们也是拓扑中相关的对象。

定义 43 给定拓扑空间 X 和一点 $x_0 \in X$,一个闭(带基点)的环路(closed based loop)是一个从参数化的圆周到 X 的连续映射:

$$\xi : [0, 2\pi] \to X$$

满足 $\xi(0)=\xi(2\pi)=x_0$。

定义 44 给定连通拓扑空间 X 和一点 $x_0 \in X$,所有闭的带基点的环路构成的空间称

为 X 的(参数化的,带基点的(parametrized based))环路空间(loop space),记为 ΩX。

评注

(i)环路空间 ΩX 上具有从闭区间$[0,2\pi]$到 X 的连续映射空间诱导而来的相对紧致开拓扑。它也有一个自然的基点:将整个$[0,2\pi]$映到 x_0的常值函数。故而容易迭代这个构造而定义 $\Omega^k X$,$k\geqslant 1$。

(ii)这里我们选择用$[0,2\pi]$来参数化圆周。如果用幅角来解释,将更为自然。我们也可以简单地选择单位区间$[0,1]$。这或许和前面对于路径的定义和后面对于同伦的定义更为一致。

命题 7 拓扑空间 X 的基本群(fundamental group),记做 $\pi_1(X)$,由 X 中的那些闭环路的类组成。这些类不能在保持基点不动的连续地形变下从一个变到另一个。

定义 45 空间 X 称为单连通的(simply-connected),如果 $\pi_1(X)$平凡。

为了定义高阶同伦群,让我们涉及一点同伦论的细节。

定义 46 给定拓扑空间 X,Y 和映射,

$$p,q:X\to Y$$

我们说 h 是映射 p,q 间的一个同伦(homotopy),如果

$$h:X\times I\to Y$$

是一个连续映射,使得 $h(x,0)=p(x)$,$h(x,1)=q(x)$。这里 I 是单位区间。在这种情况下我们记做 $p\approx q$。

定义 47 一个映射 $f:X\to Y$ 是一个同伦等价(homotopy equivalence),如果存在映射 $g:Y\to X$,使得 $g_0 f\approx id_X$,$f_0 g\approx id_Y$。

评注 这是一个等价关系。

定义 48 对于带基点 x_0 的拓扑空间 X,我们定义 $\pi_n(X)(n\geqslant 0)$为从 n 维球面 S^n 到 X 的保持基点映射的同伦等价类的集合。

评注 这和前面关于 π_0 和 π_1 的定义相容。

在同伦类和环路空间之间有一个非常好的关系。

命题 8 $\pi_n(X)=\pi_{n-1}(\Omega X)=\cdots=\pi_0(\Omega^n X)$。

评注

(i)当我们考虑 Yang-Mills 理论中的规范群(gauge group)G 时,它的基本群分类了这个理论可能出现的磁单极子(monopole)。

(ii)对于 $n\geqslant 1$,$\pi_n(X)$是一个群,群运算由连接两条环路构成一条新环路而得。另一方面,$\pi_0(X)$一般不是群。但当 X 是李群时,$\pi_0(X)$从 X 继承了一个群结构。这是因为它可以等同于 X 模掉单位连通分支而得的商群。例如,$O(3)$ 的两个连通分支可以等同于群 $\mathbf{Z}_2$ 的两个元素。行列式等于 1 的分支对应于 $\mathbf{Z}_2$ 中的 0,行列式等于 -1 的分支对应于 $\mathbf{Z}_2$ 中的 1。

(iii)对于 $n\geqslant 2$,$\pi_n(X)$总是一个阿贝尔群(abelian group)。

(iv)某些黎曼面(Riemann surface)的基本群是非阿贝尔 π_1 的例子。

(v)由于 π_1 不一定是阿贝尔群,我们用于同伦群的许多直和记号应该被更正为乘法记号。但是,在数学物理文献中,人们普遍采用加法记号。

例子

(i) $\pi_n(X\times Y)=\pi_n(X)+\pi_n(Y), n\geqslant 1$

(ii)对于球面,我们有以下结果:

$$\pi_i(S^n)=\begin{cases}0 & \text{若 } i>n\\ \mathbf{Z} & \text{若 } i=n\end{cases}$$

$$\pi_i(S^1)=0 \qquad \text{若 } i>1=0$$

$$\pi_{n+1}(S^n)=\mathbf{Z}_2 \qquad \text{若 } n\geqslant 3$$

$$\pi_{n+2}(S^n)=\mathbf{Z}_2 \qquad \text{若 } n\geqslant 2$$

$$\pi_6(S^3)=\mathbf{Z}_{12}$$

(iii)从球丛理论可以得到:

$$\pi_i(S^2)=\pi_{i-1}(S^1)+\pi_i(S^3) \qquad \text{若 } i\geqslant 2$$

$$\pi_i(S^4)=\pi_{i-1}(S^3)+\pi_i(S^7) \qquad \text{若 } i\geqslant 2$$

$$\pi_i(S^8)=\pi_{i-1}(S^7)+\pi_i(S^{15}) \qquad \text{若 } i\geqslant 2$$

第一个关系给出以下更简洁的结果:

$$\pi_i(S^3)=\pi_i(S^2) \qquad \text{若 } i\geqslant 3$$

(iv) Serre 的一个结果说,事实上,球面的所有同伦群都是有限的,除了 $\pi_n(S^n)$ 和 $\pi_{4n-1}(S^{2n}), n\geqslant 1$。

定义 49 给定一个连通空间 X,一个映射 $\pi: B\to X$ 称为一个覆叠(covering),如果(i) $\pi(B)=X$,(ii)对于每个 $x\in X$,存在 x 的一个连通开邻域 V,使得 $\pi^{-1}(V)$的每个分支在 B 中开,并且限制在每一个分支上 π 是一个同胚。空间 B 称为覆叠空间(covering space)。

例子

(i)实直线 $\mathbf{R}$ 是群 $U(1)$的一个覆叠。

(ii)群 $SU(2)$是群 $SO(3)$的一个二重覆叠。

(iii)群 $SL(2,\mathbf{C})$是洛伦兹群 $SO(1,3)$的一个二重覆叠。

(iv)$SU(2,2)$群是四维共形群(conformal group) 的一个四重覆叠。这个局部同构在 twistor 理论中非常重要。

评注

(i)通过考虑 X 中的闭环路以及它们在 B 中的覆叠,容易看出基本群 $\pi_1(X)$作用在 X 的覆叠上。如果我们进一步假设这个作用是可迁的(transitive),则有如下好的结果:X 的覆叠和 $\pi_1(X)$的正规子群(normal subgroup)1-1 对应。

(ii)给定一个连通空间 X,总存在惟一的一个单连通的覆叠空间 $\tilde{X}$,称为万有覆叠空间(universal covering space)。而且,$\tilde{X}$ 覆叠 X 的其他覆叠空间。对于高阶同伦群,有

$$\pi_n(X)=\pi_n(\tilde{X}), n\geqslant 2$$

一类非常重要的同伦群是李群的同伦群。为简单起见,我们只考虑连通群,即 $\pi_0(G)=0$。而且我们将主要考虑典型群,特别地,正交群和酉群。

命题 9 设 G 为一个连通李群,

(i)如果 G 是紧致、半单的,则 $\pi_1(G)$是有限的。这意味着 $\tilde{G}$ 还是紧致的。

(ii)$\pi_2(G)=0$。

(iii)若 G 是紧致、单、非阿贝尔的,则 $\pi_3(G)=\mathbf{Z}$。

(iv)若 G 是紧致、单连通、单的,则 $\pi_4(G)=0$ 或 $\mathbf{Z}_2$。

例子

(i)$\pi_1(SU(n))=0$。

(ii)$\pi_1(SO(n))=\mathbf{Z}_2$。

(iii)因为酉群 $U(n)$ 在拓扑上是 $SU(n)$ 和圆周 S^1 的乘积,它们的同伦群容易通过乘积公式计算。我们知道 $U(1)$ 在拓扑上是圆周,$SU(2)$ 在拓扑上是 S^3。

(iv)对于 $n\geqslant 2$,我们有

$$\pi_i(SO(3))=\pi_i(SU(2))$$
$$\pi_i(SO(5))=\pi_i(Sp(2))$$
$$\pi_i(SO(6))=\pi_i(SU(4))$$

纯属为了兴趣,并且展示这一领域的丰富,我们在表 1 中给出一些同伦群间的同构,在表 2 中给出低阶 $SU(n)$ 和 $SO(n)$ 的一些同伦群。

表 1 同伦群间的一些同构

同构	范围
$\pi_i(SO(n))\approx\pi_i(SO(m))$	$n,m\geqslant i+2$
$\pi_i(SU(n))\approx\pi_i(SU(m))$	$n,m\geqslant 1/2(i+1)$
$\pi_i(SP(n))\approx\pi_i(SP(m))$	$n,m\geqslant 1/4(i-1)$
$\pi_i(G_2)\approx\pi_i(SO(7))$	$2\leqslant i\leqslant 5$
$\pi_i(F_4)\approx\pi_i(SO(9))$	$2\leqslant i\leqslant 6$
$\pi_i(SO(9))\approx\pi_i(SO(7))$	$i\leqslant 13$

表 2 低阶 $SU(n)$ 和 $SO(n)$ 的一些同伦群

	π_4	π_5	π_6	π_7	π_8	π_9	π_{10}
$SU(2)$	$\mathbf{Z}_2$	$\mathbf{Z}_2$	$\mathbf{Z}_{12}$	$\mathbf{Z}_2$	$\mathbf{Z}_2$	$\mathbf{Z}_3$	$\mathbf{Z}_{15}$
$SU(3)$	0	$\mathbf{Z}$	$\mathbf{Z}_6$	0	$\mathbf{Z}_{12}$	$\mathbf{Z}_3$	$\mathbf{Z}_{80}$
$SU(4)$	0	$\mathbf{Z}$	0	$\mathbf{Z}$	$\mathbf{Z}_{24}$	$\mathbf{Z}_2$	$\mathbf{Z}_{120}+\mathbf{Z}_2$
$SU(5)$	0	$\mathbf{Z}$	0	$\mathbf{Z}$	0	$\mathbf{Z}$	$\mathbf{Z}_{120}$
$SU(6)$	0	$\mathbf{Z}$	0	$\mathbf{Z}$	0	$\mathbf{Z}$	$\mathbf{Z}_3$
$SO(5)$	$\mathbf{Z}_2$	$\mathbf{Z}_2$	0	$\mathbf{Z}$	0	0	$\mathbf{Z}_{120}$
$SO(6)$	0	$\mathbf{Z}$	0	$\mathbf{Z}$	$\mathbf{Z}_{24}$	$\mathbf{Z}_2$	$\mathbf{Z}_{120}+\mathbf{Z}_2$
$SO(7)$	0	0	0	$\mathbf{Z}$	$\mathbf{Z}_2+\mathbf{Z}_2$	$\mathbf{Z}_2+\mathbf{Z}_2$	$\mathbf{Z}_{24}$
$SO(8)$	0	0	0	$\mathbf{Z}+\mathbf{Z}$	$\mathbf{Z}_2+\mathbf{Z}_2+\mathbf{Z}_2$	$\mathbf{Z}_2+\mathbf{Z}_2+\mathbf{Z}_2$	$\mathbf{Z}_{24}+\mathbf{Z}_{24}$
$SO(9)$	0	0	0	$\mathbf{Z}$	$\mathbf{Z}_2+\mathbf{Z}_2$	$\mathbf{Z}_2+\mathbf{Z}_2$	$\mathbf{Z}_{24}$
$SO(10)$	0	0	0	$\mathbf{Z}$	$\mathbf{Z}_2$	$\mathbf{Z}+\mathbf{Z}_2$	$\mathbf{Z}_{12}$

附录:一个数学家的基本工具

下面是一份极为简要的单子,其中的绝大部分内容是一个数学系本科生在最初的几个星期里学到的。其余的内容是为了简要的查阅。这些记号和概念在数学文献里被广泛地使用。我们没有尽力按逻辑顺序安排内容。而且,对于结构,诸如集合、群等,人们通常可以以直接的方式定义"子结构",例如子集、子群等。所以我们将不会详细解释这一点。

集合

$AUB=\{x:x\in A$ 或 $x\in B\}$	并集(union)
$A\cap B=\{x:x\in A$ 且 $x\in B\}$	交集(intersection)
$A\backslash B=\{x:x\in A$ 且 $x\notin B\}$	余集(complement)
$A\times B=\{(x,y):x\in A\ ,y\in B\}$	笛卡儿积(Cartesian product)

映射

(1)一个映射(map,mapping) $f:A\to B$ 对 A 中的每一个元素 x 指定 B 中的一个元素 $f(x)$。

(2)一个映射 $f:A\to B$ 称为单射(injective),若 $f(x)=f(y)\Rightarrow x=y$. 它有时被称为 1-1 映射,这是一个应该避免使用的术语。

(3)一个映射 $f:A\to B$ 称为满射(surjective),若对每一个 $y\in B$,都存在 $x\in A$,使得 $y=f(x)$。它有时被称为一个"到上"(onto) 的映射。

(4)一个映射 $f:A\to B$ 称为双射(bijective),如果它既是单射又是满射。它有时也被称为 1-1 映射,这也是一个应该避免使用的术语。

(5)对于映射 $f:A\to B$,以及任意子集 $C\subseteq B$,总可以定义原像集(inverse image) $f^{-1}(C)=\{x:f(x)\in C\}\subseteq A$,尽管它可以是空集。另一方面,映射 f^{-1} 有定义当且仅当 f 是双射。

(6)一个从集合到实数或复数的映射通常叫做函数(function)。

(7)向量空间之间,特别是赋范空间(包括希尔伯特空间)之间的映射称为算子(operator)。我们通常考虑线性算子。

(8)一个从向量空间到其基域上的算子称为一个泛函(functional)。同样,我们几乎只考虑线性泛函。

关系

(1)集合 A 上的一个关系(relation)$\sim$是一个子集 $R\subseteq A\times A$。我们说 $x\sim y$,如果 $(x,y)\in R$。

(2)我们只对等价关系感兴趣。一个等价关系(equivalent relation)$\sim$是一个关系,对所有 $x,y,z\in A$,满足:

(a)$x\sim x$ ("反身性"(reflexive))

(b) $x\sim y=>y\sim x$ ("对称性"(symmetric))

(c) $x\sim y,y\sim z=>x\sim z$ ("传递性"(transitive))

(3)如果$\sim$是 A 上的一个等价关系,则对于每一个 $x\in A$,我们可以定义它的等价类

(equivalent class):

$$[x]=\{y\in A: y\sim x\}$$

可以证明等价类非空,任何两个等价类要么相等,要么不相交,所有等价类构成 A 的一个分解。子群的等价类称为陪集(coset)。

(4)等价类中的一个元素称为该类的一个代表元(representative)。

群

一个群(group)是指一个集合 G 和一个映射(称为乘法或群法则)

$$G\times G\to G$$
$$(x,y)\mapsto xy$$

满足

(1)对任意 $x,y,z\in G,(xy)z=x(yz)$("结合性"(associative))。

(2)存在一个中性元素(neutral element)(或称单位元素(identity))1 使得对任意 $x\in G,1x=x1=x$。

(3)G 中的任意元素 x 有一个逆元素(inverse) x^{-1},即 $xx^{-1}=x^{-1}x=1$。

诸如定义中的乘法的这样一个映射是二元运算(binary operation)的一个例子。注意这里我们把群法则表示为乘法。如果群是阿贝尔的,即对于任意 $x,y\in G$,有 $xy=yx$,则通常把群法则表示为加法。在这种情况下,可以把条件写成 $x+y=y+x$,并称单位元素为 0。

环

一个环 R(ring)是一个具有两个二元运算的集合,$x+y$ 称为加法(addition),xy 称为乘法(multiplication),使得

(1)R 在加法下是一个阿贝尔群。

(2)乘法是结合的。

(3)对任意 $x,y,z\in R$,有 $(x+y)z=xz+yz,x(y+z)=xy+xz$("分配性"(distributive))。

如果乘法是交换的($xy=yx$),则环称为交换的(commutative)。一个环可能含有一个乘法的单位元,此时它称为具有单位元的环(ring with unit element)。

环 R 的一个理想 I(ideal)是 R 的一个子环,且满足

$$r\in R,a\in I\Rightarrow ra\in I,ar\in I$$

我们可以以显然的方式定义左理想(left-ideal)和右理想(right-ideal)。上面定义的则称为双边理想(two-sided ideal)。

模

给定环 R,一个 R-模(R-module) M 是一个阿贝尔群,并带有一个运算 $M\times R\to R$,用乘法表示,满足对于任意 $x,y\in M,r,s\in R$

(1)$(x+y)r=xr+yr$。

(2)$x(r+s)=xr+xs$。

(3)$x(rs)=(xr)s$。

(4)$x1=x$。

我们有时使用术语右 R-模(right R-module),用以和左 R-模(left R-module)区别。左 R-模的定义是显然的。

域

一个域 F(field)是一个交换环,其中每一个非零元都是可逆的。

加法的单位元 0 是不可逆的,除非 $0=1$。所有我们通常假设一个域至少有两个元素,0 和 1。

我们遇到次数最多的域,当然是数域:有理数域、实数域和复数域。

向量空间

域 F 上的一个向量空间(vector space) V,有时也叫线性空间(linear space),是一个阿贝尔群,用加法表示,并带有一个映射 $F\times V\to V$,使得对任意 $x,y\in V,\alpha,\beta\in F$,

(1)$\alpha(x+y)=\alpha x+\alpha y$ (“线性”(linearity))。

(2)$(\alpha+\beta)x=\alpha x+\beta x$。

(3)$(\alpha\beta)x=\alpha(\beta x)$。

(4)$1x=x$。

从而一个向量空间是一个右(或左)F-模。V 中的元素称为向量(vector),F 中的元称为标量(scalar)。

代数

一个域 F 上的代数 A 是一个环,同时是 F 上的一个向量空间,使得

$$\alpha(ab)=(\alpha a)b=a(\alpha b),\alpha\in F,a,b\in A$$

注意在有些旧文献中,特别是前苏联学派的,算子代数被称为算子环。

进一步的阅读材料

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Introductory Articles

Introductory Article: Classical Mechanics

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General Principles

Classical mechanics is a theory of motions of point particles. If $\mathbf{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$ are the particle positions in a Cartesian inertial system of coordinates, the equations of motion are determined by their masses $(m_1, \ldots, m_n)$, $m_j > 0$, and by the potential energy of interaction, $V(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$, as

$$m_i \ddot{\boldsymbol{x}}_i = -\partial_{\boldsymbol{x}_i} V(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n), \quad i = 1, \ldots, n \qquad [1]$$

here $\boldsymbol{x}_i = (x_{i1}, \ldots, x_{id})$ are coordinates of the ith particle and $\partial_{\boldsymbol{x}_i}$ is the gradient $(\partial_{x_{i1}}, \ldots, \partial_{x_{id}})$; d is the space dimension (i.e., $d = 3$, usually). The potential energy function will be supposed "smooth," that is, analytic except, possibly, when two positions coincide. The latter exception is necessary to include the important cases of gravitational attraction or, when dealing with electrically charged particles, of Coulomb interaction. A basic result is that if V is bounded below, eqn [1] admits, given initial data $\boldsymbol{X}_0 = \boldsymbol{X}(0), \dot{\boldsymbol{X}}_0 = \dot{\boldsymbol{X}}(0)$, a unique global solution $t \to \boldsymbol{X}(t)$, $t \in (-\infty, \infty)$; otherwise a solution can fail to be global if and only if, in a finite time, it reaches infinity or a singularity point (i.e., a configuration in which two or more particles occupy the same point: an event called a collision).

In eqn [1], $-\partial_{\boldsymbol{x}_i} V(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$ is the force acting on the points. More general forces are often admitted. For instance, velocity-dependent friction forces: they are not considered here because of their phenomenological nature as models for microscopic phenomena which should also, in principle, be explained in terms of conservative forces (furthermore, even from a macroscopic viewpoint, they are rather incomplete models, as they should be considered together with the important heat generation phenomena that accompany them). Another interesting example of forces not corresponding to a potential are certain velocity-dependent forces like the Coriolis force (which, however, appears only in noninertial frames of reference) and the closely related Lorentz force (in electromagnetism): they could be easily accommodated in the Hamiltonian formulation of mechanics; see Appendix 2.

The action principle states that an equivalent formulation of the eqns [1] is that a motion $t \to \boldsymbol{X}_0(t)$ satisfying [1] during a time interval $[t_1, t_2]$ and leading from $\boldsymbol{X}^1 = \boldsymbol{X}_0(t_1)$ to $\boldsymbol{X}^2 = \boldsymbol{X}_0(t_2)$, renders stationary the action

$$\mathcal{A}(\{\boldsymbol{X}\}) = \int_{t_1}^{t_2} \left(\sum_{i=1}^{n} \frac{1}{2} m_i \dot{\boldsymbol{X}}_i(t)^2 - V(\boldsymbol{X}(t)) \right) \mathrm{d}t \qquad [2]$$

within the class $\mathcal{M}_{t_1,t_2}(\boldsymbol{X}^1, \boldsymbol{X}^2)$ of smooth (i.e., analytic) "motions" $t \to \boldsymbol{X}(t)$ defined for $t \in [t_1, t_2]$ and leading from $\boldsymbol{X}^1$ to $\boldsymbol{X}^2$.

The function

$$\mathcal{L}(\boldsymbol{Y}, \boldsymbol{X}) = \frac{1}{2} \sum_{i=1}^{n} m_i \boldsymbol{y}_i^2 - V(\boldsymbol{X}) \stackrel{\text{def}}{=} K(\boldsymbol{Y}) - V(\boldsymbol{X}),$$
$$\boldsymbol{Y} = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n)$$

is called the Lagrangian function and the action can be written as

$$\int_{t_1}^{t_2} \mathcal{L}(\dot{\boldsymbol{X}}(t), \boldsymbol{X}(t))\, \mathrm{d}t$$

The quantity $K(\dot{\boldsymbol{X}}(t))$ is called kinetic energy and motions satisfying [1] conserve energy as time t varies, that is,

$$K(\dot{\boldsymbol{X}}(t)) + V(\boldsymbol{X}(t)) = E = \text{const.} \qquad [3]$$

Hence the action principle can be intuitively thought of as saying that motions proceed by keeping constant the energy, sum of the kinetic and potential energies, while trying to share as evenly as possible their (average over time) contribution to the energy.

In the special case in which V is translation invariant, motions conserve linear momentum $\boldsymbol{Q} \stackrel{\text{def}}{=} \sum_i m_i \dot{\boldsymbol{x}}_i$; if V

is rotation invariant around the origin O, motions conserve angular momentum $\boldsymbol{M} \stackrel{\text{def}}{=} \sum_i m_i \boldsymbol{x}_i \wedge \dot{\boldsymbol{x}}_i$, where $\wedge$ denotes the vector product in $\mathbb{R}^d$, that is, it is the tensor $(\boldsymbol{a} \wedge \boldsymbol{b})_{ij} = a_i b_j - b_i a_j, i, j = 1, \ldots, d$: if the dimension $d = 3$ the $\boldsymbol{a} \wedge \boldsymbol{b}$ will be naturally regarded as a vector. More generally, to any continuous symmetry group of the Lagrangian correspond conserved quantities: this is formalized in the *Noether theorem*.

It is convenient to think that the scalar product in $\mathbb{R}^{dn}$ is defined in terms of the ordinary scalar product in $\mathbb{R}^d$, $\boldsymbol{a} \cdot \boldsymbol{b} = \sum_{j=1}^{d} a_j b_j$, by $(\boldsymbol{v}, \boldsymbol{w}) = \sum_{i=1}^{n} m_i \boldsymbol{v}_i \cdot \boldsymbol{w}_i$: so that kinetic energy and line element $\mathrm{d}s$ can be written as $K(\dot{\boldsymbol{X}}) = \frac{1}{2}(\dot{\boldsymbol{X}}, \dot{\boldsymbol{X}})$ and $\mathrm{d}s^2 = \sum_{i=1}^{n} m_i \, \mathrm{d}\boldsymbol{x}_i^2$, respectively. Therefore, the metric generated by the latter scalar product can be called *kinetic energy metric*.

The interest of the kinetic metric appears from the *Maupertuis' principle* (equivalent to [1]): the principle allows us to identify the trajectory traced in $\mathbb{R}^d$ by a motion that leads from $\boldsymbol{X}^1$ to $\boldsymbol{X}^2$ moving with energy E. Parametrizing such trajectories as $\tau \to \boldsymbol{X}(\tau)$ by a parameter τ varying in [0, 1] so that the line element is $\mathrm{d}s^2 = (\partial_\tau \boldsymbol{X}, \partial_\tau \boldsymbol{X}) \, \mathrm{d}\tau^2$, the principle states that the trajectory of a motion with energy E which leads from $\boldsymbol{X}^1$ to $\boldsymbol{X}^2$ makes stationary, among the analytic curves $\boldsymbol{\xi} \in \mathcal{M}_{0,1}(\boldsymbol{X}^1, \boldsymbol{X}^2)$, the function

$$L(\boldsymbol{\xi}) = \int_{\boldsymbol{\xi}} \sqrt{E - V(\boldsymbol{\xi}(s))} \, \mathrm{d}s \qquad [4]$$

so that the possible trajectories traced by the solutions of [1] in $\mathbb{R}^{nd}$ and with energy E can be identified with the geodesics of the metric $\mathrm{d}m^2 \stackrel{\text{def}}{=} (E - V(\boldsymbol{X})) \cdot \mathrm{d}s^2$.

For more details, the reader is referred to Landau and Lifshitz (1976) and Gallavotti (1983).

Constraints

Often particles are subject to constraints which force the motion to take place on a surface $M \subset \mathbb{R}^{nd}$, i.e., $\boldsymbol{X}(t)$ is forced to be a point on the manifold M. A typical example is provided by rigid systems in which motions are subject to forces which keep the mutual distances of the particles constant: $|\boldsymbol{x}_i - \boldsymbol{x}_j| = \rho_{ij}$, with ρ_{ij} time-independent positive quantities. In essentially all cases, the forces that imply constraints, called constraint reactions, are velocity dependent and, therefore, are not in the class of conservative forces considered here, cf. [1]. Hence, from a fundamental viewpoint admitting only conservative forces, constrained systems should be regarded as idealizations of systems subject to conservative forces which approximately imply the constraints.

In general, the ℓ-dimensional manifold M will not admit a global system of coordinates: however, it will be possible to describe points in the vicinity of any $\boldsymbol{X}^0 \in M$ by using $N = nd$ coordinates $q = (q_1, \ldots, q_\ell, q_{\ell+1}, \ldots, q_N)$ varying in an open ball B_{X^0}: $\boldsymbol{X} = \boldsymbol{X}(q_1, \ldots, q_\ell, q_{\ell+1}, \ldots, q_N)$.

The q-coordinates can be chosen well adapted to the surface M and to the kinetic metric, i.e., so that the points of M are identified by $q_{\ell+1} = \cdots = q_N = 0$ (which is the meaning of "adapted"); furthermore, infinitesimal displacements $(0, \ldots, 0, \mathrm{d}\varepsilon_{\ell+1}, \ldots, \mathrm{d}\varepsilon_N)$ out of a point $\boldsymbol{X}^0 \in M$ are orthogonal to M (in the kinetic metric) and have a length independent of the position of $\boldsymbol{X}^0$ on M (which is the meaning of "well adapted" to the kinetic metric).

Motions constrained on M arise when the potential V has the form

$$V(\boldsymbol{X}) = V_a(\boldsymbol{X}) + \lambda W(\boldsymbol{X}) \qquad [5]$$

where W is a smooth function which reaches its minimum value, say equal to 0, precisely on the manifold M while V_a is another smooth potential. The factor $\lambda > 0$ is a parameter called the rigidity of the constraint.

A particularly interesting case arises when the level surfaces of W also have the geometric property of being "parallel" to the surface M: in the precise sense that the matrix $\partial^2_{q_i q_j} W(\boldsymbol{X})$, $i, j > \ell$ is positive definite and $\boldsymbol{X}$-independent, for all $\boldsymbol{X} \in M$, in a system of coordinates well adapted to the kinetic metric.

A potential W with the latter properties can be called an approximately ideal constraint reaction. In fact, it can be proved that, given an initial datum $\boldsymbol{X}^0 \in M$ with velocity $\dot{\boldsymbol{X}}^0$ tangent to M, i.e., given an initial datum whose coordinates in a local system of coordinates are $(q_0, 0)$ and $(\dot{q}_0, 0)$ with $q_0 = (q_{01}, \ldots, q_{0\ell})$ and $\dot{q}_0 = (\dot{q}_{01}, \ldots, \dot{q}_{0\ell})$, the motion generated by [1] with V given by [5] is a motion $t \to \boldsymbol{X}_\lambda(t)$ which

1. as $\lambda \to \infty$ tends to a motion $t \to \boldsymbol{X}_\infty(t)$;
2. as long as $\boldsymbol{X}_\infty(t)$ stays in the vicinity of the initial data, say for $0 \le t \le t_1$, so that it can be described in the above local adapted coordinates, its coordinates have the form $t \to (q(t), 0) = (q_1(t), \ldots, q_\ell(t), 0, \ldots, 0)$: that is, it is a motion developing on the constraint surface M; and
3. the curve $t \to \boldsymbol{X}_\infty(t)$, $t \in [0, t_1]$, as an element of the space $\mathcal{M}_{0,t_1}(\boldsymbol{X}^0, \boldsymbol{X}_\infty(t_1))$ of analytic curves on M connecting $\boldsymbol{X}^0$ to $\boldsymbol{X}_\infty(t_1)$, renders the action

$$A(\boldsymbol{X}) = \int_0^{t_1} \left(K(\dot{\boldsymbol{X}}(t)) - V_a(\boldsymbol{X}(t))\right) \mathrm{d}t \qquad [6]$$

stationary.

The latter property can be formulated "intrinsically," that is, referring only to M as a surface, via the restriction of the metric ds^2 to line elements $ds = (dq_1, \ldots, dq_\ell, 0, \ldots, 0)$ tangent to M at the point $\mathbf{X} = (q_0, 0, \ldots, 0) \in M$; we write $ds^2 = \sum_{i,j}^{1,\ell} g_{ij}(q) \times dq_i\, dq_j$. The $\ell \times \ell$ symmetric positive-definite matrix g can be called the *metric* on M induced by the kinetic energy. Then the action in [6] can be written as

$$\mathcal{A}(q) = \int_0^{t_1} \left(\frac{1}{2} \sum_{i,j}^{1,\ell} g_{ij}(q(t)) \dot{q}_i(t) \dot{q}_j(t) - \overline{V}_a(q(t)) \right) dt \qquad [7]$$

where $\overline{V}_a(q) \stackrel{\text{def}}{=} V_a(\mathbf{X}(q_1, \ldots, q_\ell, 0, \ldots, 0))$: the function

$$\mathcal{L}(\eta, q) \stackrel{\text{def}}{=} \frac{1}{2} \sum_{i,j}^{1,\ell} g_{ij}(q) \eta_i \eta_j - \overline{V}_a(q) \equiv \frac{1}{2} g(q)\eta \cdot \eta - \overline{V}_a(q) \qquad [8]$$

is called the constrained Lagrangian of the system.

An important property is that the constrained motions conserve the energy defined as $E = \frac{1}{2}(g(q)\dot{q}, \dot{q}) + \overline{V}_a(q)$; see next section.

The constrained motion $\mathbf{X}_\infty(t)$ of energy E satisfies the Maupertuis' principle in the sense that the curve on M on which the motion develops renders

$$L(\xi) = \int_\xi \sqrt{E - V_a(\xi(s))}\, ds \qquad [9]$$

stationary among the (smooth) curves that develop on M connecting two fixed values $\mathbf{X}_1$ and $\mathbf{X}_2$. In the particular case in which $\ell = n$ this is again Maupertuis' principle for unconstrained motions under the potential $V(\mathbf{X})$. In general, ℓ is called the number of degrees of freedom because a complete description of the initial data requires 2ℓ coordinates $q(0), \dot{q}(0)$.

If W is minimal on M but the condition on W of having level surfaces parallel to M is not satisfied, i.e., if W is not an approximate ideal constraint reaction, it still remains true that the limit motion $\mathbf{X}_\infty(t)$ takes place on M. However, in general, it will not satisfy the above variational principles. For this reason, motions arising as limits (as $\lambda \to \infty$) of motions developing under the potential [5] with W having minimum on M and level curves parallel (in the above sense) to M are called ideally constrained motions or motions subject by ideal constraints to the surface M.

As an example, suppose that W has the form $W(\mathbf{X}) = \sum_{i,j \in \mathcal{P}} w_{ij}(|\mathbf{x}_i - \mathbf{x}_j|)$ with $w_{ij}(|\xi|) \geq 0$ an analytic function vanishing only when $|\xi| = \rho_{ij}$ for i, j in some set of pairs $\mathcal{P}$ and for some given distances ρ_{ij} (e.g., $w_{ij}(\xi) = (\xi^2 - \rho_{ij}^2)^2 \gamma, \gamma > 0$). Then W can be shown to satisfy the mentioned conditions and therefore, the so constrained motions $\mathbf{X}_\infty(t)$ of the body satisfy the variational principles mentioned in connection with [7] and [9]: in other words, the above natural way of realizing a rather general rigidity constraint is ideal.

The modern viewpoint on the physical meaning of the constraint reactions is as follows: looking at motions in an inertial Cartesian system, it will appear that the system is subject to the applied forces with potential $V_a(\mathbf{X})$ and to constraint forces which are defined as the differences $\mathbf{R}_i = m_i \ddot{\mathbf{x}}_i + \partial_{\mathbf{x}_i} V_a(\mathbf{X})$. The latter reflect the action of the forces with potential $\lambda W(\mathbf{X})$ in the limit of infinite rigidity ($\lambda \to \infty$).

In applications, sometimes the action of a constraint can be regarded as ideal: the motion will then verify the variational principles mentioned and $\mathbf{R}$ can be computed as the differences between the $m_i \ddot{\mathbf{x}}_i$ and the active forces $-\partial_{\mathbf{x}_i} V_a(\mathbf{X})$. In dynamics problems it is, however, a very difficult and important matter, particularly in engineering, to judge whether a system of particles can be considered as subject to ideal constraints: this leads to important decisions in the construction of machines. It simplifies the calculations of the reactions and fatigue of the materials but a misjudgment can have serious consequences about stability and safety. For statics problems, the difficulty is of lower order: usually assuming that the constraint reaction is ideal leads to an overestimate of the requirements for stability of equilibria. Hence, employing the action principle to statics problems, where it constitutes the principle of *virtual work*, generally leads to economic problems rather than to safety issues. Its discovery even predates Newtonian mechanics.

We refer the reader to Arnol'd (1989) and Gallavotti (1983) for more details.

Lagrange and Hamilton Forms of the Equations of Motion

The stationarity condition for the action $\mathcal{A}(q)$, cf. [7], [8], is formulated in terms of the Lagrangian $\mathcal{L}(\eta, \xi)$, see [8], by

$$\frac{d}{dt} \partial_{\eta_i} \mathcal{L}(\dot{q}(t), q(t)) = \partial_{\xi_i} \mathcal{L}(\dot{q}(t), q(t)), \quad i = 1, \ldots, \ell \qquad [10]$$

which is a second-order differential equation called the Lagrangian equation of motion. It can be cast in "normal form": for this purpose, adopting the convention of "summation over repeated indices," introduce the "generalized momenta"

$$p_i \stackrel{\text{def}}{=} g(q)_{ij} \dot{q}_j, \quad i = 1, \ldots, \ell \qquad [11]$$

Since $g(q) > 0$, the motions $t \to q(t)$ and the corresponding velocities $t \to \dot{q}(t)$ can be described equivalently by $t \to (q(t), p(t))$: and the equations of motion [10] become the first-order equations

$$\dot{q}_i = \partial_{p_i}\mathcal{H}(p,q), \qquad \dot{p}_i = -\partial_{q_i}H(p,q) \qquad [12]$$

where the function $\mathcal{H}$, called the Hamiltonian of the system, is defined by

$$\mathcal{H}(p,q) \stackrel{\text{def}}{=} \tfrac{1}{2}(g(q)^{-1}p,p) + \overline{V}_a(q) \qquad [13]$$

Equations [12], regarded as equations of motion for phase space points (p,q), are called Hamilton equations. In general, q are local coordinates on M and motions are specified by giving $q, \dot{q}$ or p, q.

Looking for a coordinate-free representation of motions consider the pairs X, Y with $X \in M$ and Y a vector $Y \in T_X$ tangent to M at the point X. The collection of pairs (Y,X) is denoted $T(M) = \cup_{X\in M}(T_X \times \{X\})$ and a motion $t \to (\dot{X}(t), X(t)) \in T(M)$ in local coordinates is represented by $(\dot{q}(t), q(t))$. The space $T(M)$ can be called the space of initial data for Lagrange's equations of motion: it has 2ℓ dimensions (also known as the "tangent bundle" of M).

Likewise, the space of initial data for the Hamilton equations will be denoted $T^*(M)$ and it consists of pairs X, P with $X \in M$ and $P = g(X)Y$ with Y a vector tangent to M at X. The space $T^*(M)$ is called the phase space of the system: it has 2ℓ dimensions (and it is occasionally called the "cotangent bundle" of M).

Immediate consequence of [12] is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(p(t), q(t)) \equiv 0$$

and it means that $\mathcal{H}(p(t), q(t))$ is constant along the solutions of [12]. Noting that $\mathcal{H}(p,q) = (1/2)(g(q)\ \dot{q}, \dot{q}) + \overline{V}_a(q)$ is the sum of the kinetic and potential energies, it follows that the conservation of $\mathcal{H}$ along solutions means energy conservation in presence of ideal constraints.

Let S_t be the flow generated on the phase space variables (p,q) by the solutions of the equations of motion [12], that is, let $t \to S_t(p,q) \equiv (p(t), q(t))$ denote a solution of [12] with initial data (p,q). Then a (measurable) set Δ in phase space evolves in time t into a new set $S_t\Delta$ with the same volume: this is obvious because the Hamilton equations [12] have manifestly zero divergence ("Liouville's theorem").

The Hamilton equations also satisfy a variational principle, called the Hamilton action principle: that is, if $\mathcal{M}_{t_1,t_2}((p_1,q_1),(p_2,q_2);M)$ denotes the space of the analytic functions $\varphi : t \to (\pi(t), \kappa(t))$ which in the time interval $[t_1, t_2]$ lead from (p_1,q_1) to (p_2,q_2), then the condition that $\varphi_0(t) = (p(t), q(t))$ satisfies [12] can be equivalently formulated by requiring that the function

$$\mathcal{A}_{\mathcal{H}}(\varphi) \stackrel{\text{def}}{=} \int_{t_1}^{t_2} \Big(\pi(t)\cdot\dot{\kappa}(t) - \mathcal{H}(\pi(t),\kappa(t))\Big)\,\mathrm{d}t \qquad [14]$$

be stationary for $\varphi = \varphi_0$: in fact, eqns [12] are the stationarity conditions for the Hamilton action [14] on $\mathcal{M}_{t_0,t_1}((p_1,q_1),(p_2,q_2);M)$. And, since the derivatives of $\pi(t)$ do not appear in [14], stationarity is even achieved in the larger space $\mathcal{M}_{t_1,t_2}(q_1,q_2;M)$ of the motions $\varphi : t \to (\pi(t), \kappa(t))$ leading from q_1 to q_2 without any restriction on the initial and final momenta p_1, p_2 (which, therefore, cannot be prescribed *a priori* independently of q_1, q_2). If the prescribed data p_1, q_1, p_2, q_2 are not compatible with the equations of motion (e.g., $H(p_1,q_2) \neq H(p_2,q_2)$), then the action functional has no stationary trajectory in $\mathcal{M}_{t_1,t_2}((p_1,q_1),(p_2q_2);M)$.

For more details, the reader is referred to Landau and Lifshitz (1976), Arnol'd (1989), and Gallavotti (1983).

Canonical Transformations of Phase Space Coordinates

The Hamiltonian form, [13], of the equations of motion turns out to be quite useful in several problems. It is, therefore, important to remark that it is invariant under a special class of transformations of coordinates, called canonical transformations.

Consider a local change of coordinates on phase space, i.e., a smooth, smoothly invertible map $\mathcal{C}(\pi,\kappa) = (\pi',\kappa')$ between an open set U in the phase space of a Hamiltonian system with ℓ degrees of freedom, into an open set U' in a 2ℓ-dimensional space. The change of coordinates is said to be *canonical* if for any solution $t \to (\pi(t), \kappa(t))$ of equations like [12], for any Hamiltonian $\mathcal{H}(\pi,\kappa)$ defined on U, the $\mathcal{C}$–image $t \to (\pi'(t), \kappa'(t)) = \mathcal{C}(\pi(t), \kappa(t))$ is a solution of [12] with the "same" Hamiltonian, that is, with Hamiltonian $\mathcal{H}'(\pi',\kappa') \stackrel{\text{def}}{=} \mathcal{H}(\mathcal{C}^{-1}(\pi',\kappa'))$.

The condition that a transformation of coordinates is canonical is obtained by using the arbitrariness of the function $\mathcal{H}$ and is simply expressed as a necessary and sufficient property of the Jacobian L,

$$L = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$
$$A_{ij} = \partial_{\pi_j}\pi'_i, \quad B_{ij} = \partial_{\kappa_j}\pi'_i, \qquad [15]$$
$$C_{ij} = \partial_{\pi_j}\kappa'_i, \quad D_{ij} = \partial_{\kappa_j}\kappa'_i$$

where $i, j = 1, \ldots, \ell$. Let

$$E = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

denote the $2\ell \times 2\ell$ matrix formed by four $\ell \times \ell$ blocks, equal to the 0 matrix or, as indicated, to the $\pm$(identity matrix); then, if a superscript T denotes matrix transposition, the condition that the map be canonical is that

$$L^{-1} = EL^{\mathrm{T}}E^{\mathrm{T}} \text{ or } L^{-1} = \begin{pmatrix} D^{\mathrm{T}} & -B^{\mathrm{T}} \\ -C^{\mathrm{T}} & A^{\mathrm{T}} \end{pmatrix} \qquad [16]$$

which immediately implies that $\det L = \pm 1$. In fact, it is possible to show that [16] implies $\det L = 1$. Equation [16] is equivalent to the four relations $AD^{\mathrm{T}} - BC^{\mathrm{T}} = 1$, $-AB^{\mathrm{T}} + BA^{\mathrm{T}} = 0, CD^{\mathrm{T}} - DC^{\mathrm{T}} = 0,$ and $-CB^{\mathrm{T}} + DA^{\mathrm{T}} = 1$. More explicitly, since the first and the fourth relations coincide, these can be expressed as

$$\{\pi'_i, \kappa'_j\} = \delta_{ij}, \ \{\pi'_i, \pi'_j\} = 0, \ \{\kappa'_i, \kappa'_j\} = 0 \qquad [17]$$

where, for any two functions $F(\boldsymbol{\pi}, \boldsymbol{\kappa})$, $G(\boldsymbol{\pi}, \boldsymbol{\kappa})$, the *Poisson bracket* is

$$\{F, G\}(\boldsymbol{\pi}, \boldsymbol{\kappa}) \stackrel{\text{def}}{=} \sum_{k=1}^{\ell} (\partial_{\pi_k} F(\boldsymbol{\pi}, \boldsymbol{\kappa}) \partial_{\kappa_k} G(\boldsymbol{\pi}, \boldsymbol{\kappa}) - \partial_{\kappa_k} F(\boldsymbol{\pi}, \boldsymbol{\kappa})\, \partial_{\pi_k} G(\boldsymbol{\pi}, \boldsymbol{\kappa})) \qquad [18]$$

The latter satisfies *Jacobi's identity*: $\{\{F, G\}, Q\} + \{\{G, Q\}, F\} + \{\{Q, F\}, G\} = 0$, for any three functions F, G, Q on the phase space. It is quite useful to remark that if $t \to (\boldsymbol{p}(t), \boldsymbol{q}(t)) = S_t(\boldsymbol{p}, \boldsymbol{q})$ is a solution to Hamilton equations with Hamiltonian $\mathcal{H}$ then, given any observable $F(\boldsymbol{p}, \boldsymbol{q})$, it "evolves" as $F(t) \stackrel{\text{def}}{=} F(\boldsymbol{p}(t), \boldsymbol{q}(t))$ satisfying

$$\partial_t F(\boldsymbol{p}(t), \boldsymbol{q}(t)) = \{\mathcal{H}, F\}(\boldsymbol{p}(t), \boldsymbol{q}(t))$$

Requiring the latter identity to hold for all observables F is equivalent to requiring that the $t \to (\boldsymbol{p}(t), \boldsymbol{q}(t))$ be a solution of Hamilton's equations for $\mathcal{H}$.

Let $\mathcal{C} : U \longleftrightarrow U'$ be a smooth, smoothly invertible transformation between two open 2ℓ-dimensional sets: $\mathcal{C}(\boldsymbol{\pi}, \boldsymbol{\kappa}) = (\boldsymbol{\pi}', \boldsymbol{\kappa}')$. Suppose that there is a function $\Phi(\boldsymbol{\pi}', \boldsymbol{\kappa})$ defined on a suitable domain W such that

$$\mathcal{C}(\boldsymbol{\pi}, \boldsymbol{\kappa}) = (\boldsymbol{\pi}', \boldsymbol{\kappa}') \ \Rightarrow \ \begin{cases} \boldsymbol{\pi} = \partial_{\boldsymbol{\kappa}} \Phi(\boldsymbol{\pi}', \boldsymbol{\kappa}) \\ \boldsymbol{\kappa}' = \partial_{\boldsymbol{\pi}'} \Phi(\boldsymbol{\pi}', \boldsymbol{\kappa}) \end{cases} \qquad [19]$$

then $\mathcal{C}$ is canonical. This is because [19] implies that if $\boldsymbol{\kappa}, \boldsymbol{\pi}'$ are varied and if $\boldsymbol{\pi}, \boldsymbol{\kappa}', \boldsymbol{\pi}', \boldsymbol{\kappa}$ are related by $\mathcal{C}(\boldsymbol{\pi}, \boldsymbol{\kappa}) = (\boldsymbol{\pi}', \boldsymbol{\kappa}')$, then $\boldsymbol{\pi} \cdot \mathrm{d}\boldsymbol{\kappa} + \boldsymbol{\kappa}' \cdot \mathrm{d}\boldsymbol{\pi}' = \mathrm{d}\Phi(\boldsymbol{\pi}', \boldsymbol{\kappa})$, which implies that

$$\boldsymbol{\pi} \cdot \mathrm{d}\boldsymbol{\kappa} - \mathcal{H}(\boldsymbol{\pi}, \boldsymbol{\kappa})\mathrm{d}t \equiv \boldsymbol{\pi}' \cdot \mathrm{d}\boldsymbol{\kappa}' - \mathcal{H}(\mathcal{C}^{-1}(\boldsymbol{\pi}', \boldsymbol{\kappa}'))\mathrm{d}t + \mathrm{d}\Phi(\boldsymbol{\pi}', \boldsymbol{\kappa}) - \mathrm{d}(\boldsymbol{\pi}' \cdot \boldsymbol{\kappa}') \qquad [20]$$

It means that the Hamiltonians $\mathcal{H}(\boldsymbol{p}, \boldsymbol{q})$ and $\mathcal{H}'(\boldsymbol{p}', \boldsymbol{q}') \stackrel{\text{def}}{=} \mathcal{H}(\mathcal{C}^{-1}(\boldsymbol{p}', \boldsymbol{q}'))$ have Hamilton actions $\mathcal{A}_{\mathcal{H}}$ and $\mathcal{A}_{\mathcal{H}'}$ differing by a constant, if evaluated on corresponding motions $(\boldsymbol{p}(t), \boldsymbol{q}(t))$ and $(\boldsymbol{p}'(t), \boldsymbol{q}'(t)) = \mathcal{C}(\boldsymbol{p}(t), \boldsymbol{q}(t))$.

The constant depends only on the initial and final values $(\boldsymbol{p}(t_1), \boldsymbol{q}(t_1))$ and $(\boldsymbol{p}(t_2), \boldsymbol{q}(t_2))$ and, respectively, $(\boldsymbol{p}'(t_1), \boldsymbol{q}'(t_1))$ and $(\boldsymbol{p}'(t_2), \boldsymbol{q}'(t_2))$ so that if $(\boldsymbol{p}(t), \boldsymbol{q}(t))$ makes $\mathcal{A}_{\mathcal{H}}$ extreme, then $(\boldsymbol{p}'(t), \boldsymbol{q}'(t)) = \mathcal{C}(\boldsymbol{p}(t), \boldsymbol{q}(t))$ also makes $\mathcal{A}_{\mathcal{H}'}$ extreme.

Hence, if $t \to (\boldsymbol{p}(t), \boldsymbol{q}(t))$ solves the Hamilton equations with Hamiltonian $\mathcal{H}(\boldsymbol{p}, \boldsymbol{q})$ then the motion $t \to (\boldsymbol{p}'(t), \boldsymbol{q}'(t)) = \mathcal{C}(\boldsymbol{p}(t), \boldsymbol{q}(t))$ solves the Hamilton equations with Hamiltonian $\mathcal{H}'(\boldsymbol{p}', \boldsymbol{q}') = \mathcal{H}(\mathcal{C}^{-1}(\boldsymbol{p}', \boldsymbol{q}'))$ no matter which it is: therefore, the transformation is canonical. The function Φ is called its generating function.

Equation [19] provides a way to construct canonical maps. Suppose that a function $\Phi(\boldsymbol{\pi}', \boldsymbol{\kappa})$ is given and defined on some domain W; then setting

$$\begin{cases} \boldsymbol{\pi} = \partial_{\boldsymbol{\kappa}} \Phi(\boldsymbol{\pi}', \boldsymbol{\kappa}) \\ \boldsymbol{\kappa}' = \partial_{\boldsymbol{\pi}'} \Phi(\boldsymbol{\pi}', \boldsymbol{\kappa}) \end{cases}$$

and inverting the first equation in the form $\boldsymbol{\pi}' = \boldsymbol{\Xi}(\boldsymbol{\pi}, \boldsymbol{\kappa})$ and substituting the value for $\boldsymbol{\pi}'$ thus obtained, in the second equation, a map $\mathcal{C}(\boldsymbol{\pi}, \boldsymbol{\kappa}) = (\boldsymbol{\pi}', \boldsymbol{\kappa}')$ is defined on some domain (where the mentioned operations can be performed) and if such domain is open and not empty then $\mathcal{C}$ is a canonical map.

For similar reasons, if $\Gamma(\boldsymbol{\kappa}, \boldsymbol{\kappa}')$ is a function defined on some domain then setting $\boldsymbol{\pi} = \partial_{\boldsymbol{\kappa}} \Gamma(\boldsymbol{\kappa}, \boldsymbol{\kappa}')$, $\boldsymbol{\pi}' = -\partial_{\boldsymbol{\kappa}'} \Gamma(\boldsymbol{\kappa}, \boldsymbol{\kappa}')$ and solving the first relation to express $\boldsymbol{\kappa}' = \boldsymbol{\Delta}(\boldsymbol{\pi}, \boldsymbol{\kappa})$ and substituting in the second relation a map $(\boldsymbol{\pi}', \boldsymbol{\kappa}') = \mathcal{C}(\boldsymbol{\pi}, \boldsymbol{\kappa})$ is defined on some domain (where the mentioned operations can be performed) and if such domain is open and not empty then $\mathcal{C}$ is a canonical map.

Likewise, canonical transformations can be constructed starting from *a priori* given functions $F(\boldsymbol{\pi}, \boldsymbol{\kappa}')$ or $G(\boldsymbol{\pi}, \boldsymbol{\pi}')$. And the most general canonical map can be generated locally (i.e., near a given point in phase space) by a single one of the above four ways, possibly composed with a few "trivial" canonical maps in which one pair of coordinates (π_i, κ_i) is transformed into $(-\kappa_i, \pi_i)$. The necessity of also including the trivial maps can be traced to the existence of homogeneous canonical maps, that is, maps such that $\boldsymbol{\pi} \cdot \mathrm{d}\boldsymbol{\kappa} = \boldsymbol{\pi}' \cdot \mathrm{d}\boldsymbol{\kappa}'$ (e.g., the identity map, see below or [49] for nontrivial examples) which are action preserving hence canonical, but which evidently cannot be generated by a function $\Phi(\boldsymbol{\kappa}, \boldsymbol{\kappa}')$ although they can be generated by a function depending on $\boldsymbol{\pi}', \boldsymbol{\kappa}$.

Simple examples of homogeneous canonical maps are maps in which the coordinates q are changed into $q' = R(q)$ and, correspondingly, the p's are transformed as $p' = (\partial_q R(q))^{-1\,\mathrm{T}} p$, linearly: indeed, this map is generated by the function $F(p', q) \stackrel{\text{def}}{=} p' \cdot R(q)$.

For instance, consider the map "Cartesian–polar" coordinates $(q_1, q_2) \longleftrightarrow (\rho, \theta)$ with (ρ, θ) the polar coordinates of q (namely $\rho = \sqrt{q_1^2 + q_2^2}$, $\theta =$ arctan (q_2/q_1)) and let $n \stackrel{\text{def}}{=} q/|q| = (n_1, n_2)$ and $t = (-n_2, n_1)$. Setting $p_\rho \stackrel{\text{def}}{=} p \cdot n$, $p_\theta \stackrel{\text{def}}{=} \rho p \cdot t$, the map $(p_1, p_2, q_1, q_2) \longleftrightarrow (p_\rho, p_\theta, \rho, \theta)$ is homogeneous canonical (because $p \cdot dq = p \cdot n\, d\rho + p \cdot t \rho\, d\theta = p_\rho\, d\rho + p_\theta\, d\theta$).

As a further example, any area-preserving map $(p, q) \longleftrightarrow (p', q')$ defined on an open region of the plane $\mathbb{R}^2$ is canonical: because in this case the matrices A, B, C, D are just numbers, which satisfy $AD - BC = 1$ and, therefore, [16] holds.

For more details, the reader is referred to Landau and Lifshitz (1976) and Gallavotti (1983).

Quadratures

The simplest mechanical systems are integrable by quadratures. For instance, the Hamiltonian on $\mathbb{R}^2$,

$$\mathcal{H}(p, q) = \frac{1}{2m} p^2 + V(q) \qquad [21]$$

generates a motion $t \to q(t)$ with initial data $q_0, \dot{q}_0$ such that $\mathcal{H}(p_0, q_0) = E$, i.e., $\frac{1}{2} m \dot{q}_0^2 + V(q_0) = E$, satisfying

$$\dot{q}(t) = \pm \sqrt{\frac{2}{m}(E - V(q(t)))}$$

If the equation $E = V(q)$ has only two solutions $q_-(E) < q_+(E)$ and $|\partial_q V(q_\pm(E))| > 0$, the motion is periodic with period

$$T(E) = 2 \int_{q_-(E)}^{q_+(E)} \frac{dx}{\sqrt{(2/m)(E - V(x))}} \qquad [22]$$

The special solution with initial data $q_0 = q_-(E)$, $\dot{q}_0 = 0$ will be denoted $Q(t)$, and it is an analytic function (by the general regularity theorem on ordinary differential equations). For $0 \le t \le T/2$ or for $T/2 \le t \le T$ it is given, respectively, by

$$t = \int_{q_-(E)}^{Q(t)} \frac{dx}{\sqrt{(2/m)(E - V(x))}} \qquad [23a]$$

or

$$t = \frac{T}{2} - \int_{q_+(E)}^{Q(t)} \frac{dx}{\sqrt{(2/m)(E - V(x))}} \qquad [23b]$$

The most general solution with energy E has the form $q(t) = Q(t_0 + t)$, where t_0 is defined by $q_0 = Q(t_0)$, $\dot{q}_0 = \dot{Q}(t_0)$, i.e., it is the time needed for the "standard solution" $Q(t)$ to reach the initial data for the new motion.

If the derivative of V vanishes in one of the extremes or if at least one of the two solutions $q_\pm(E)$ does not exist, the motion is not periodic and it may be unbounded: nevertheless, it is still expressible via integrals of the type [22]. If the potential V is periodic in q and the variable q is considered to be varying on a circle then essentially all solutions are periodic: exceptions can occur if the energy E has a value such that $V(q) = E$ admits a solution where V has zero derivative.

Typical examples are the harmonic oscillator, the pendulum, and the Kepler oscillator: whose Hamiltonians, if m, ω, g, h, G, k are positive constants, are, respectively,

$$\frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2$$
$$\frac{p^2}{2m} + mg\left(1 - \cos\frac{q}{h}\right) \qquad [24]$$
$$\frac{p^2}{2m} - mk\frac{1}{|q|} + m\frac{G^2}{2q^2}$$

the Kepler oscillator Hamiltonian has a potential which is singular at $q = 0$ but if $G \neq 0$ the energy conservation forbids too close an approach to $q = 0$ and the singularity becomes irrelevant.

The integral in [23] is called a *quadrature* and the systems in [21] are therefore *integrable by quadratures*. Such systems, at least when the motion is periodic, are best described in new coordinates in which periodicity is more manifest. Namely when $V(q) = E$ has only two roots $q_\pm(E)$ and $\mp V'(q_\pm(E)) > 0$ the *energy–time coordinates* can be used by replacing $q, \dot{q}$ or p, q by E, τ, where τ is the time needed for the standard solution $t \to Q(t)$ to reach the given data, that is, $Q(\tau) = q, \dot{Q}(\tau) = \dot{q}$. In such coordinates, the motion is simply $(E, \tau) \to (E, \tau + t)$ and, of course, the variable τ has to be regarded as varying on a circle of radius $T/2\pi$. The E, τ variables are a kind of polar coordinates, as can be checked by drawing the curves of constant E, "energy levels," in the plane p, q in the cases in [24]; see **Figure 1**.

In the harmonic oscillator case, all trajectories are periodic. In the pendulum case, all motions are periodic except the ones which separate the oscillatory motions (the closed curves in the second drawing) from the rotatory motions (the apparently open curves) which, in fact, are on closed curves as well if the q coordinate, that is, the vertical

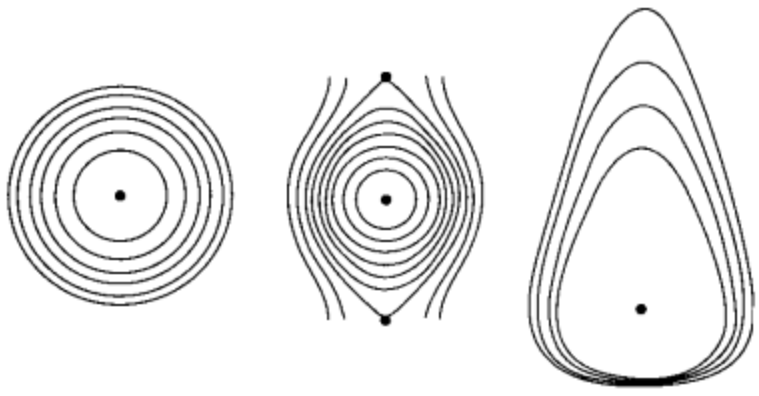

Figure 1 The energy levels of the harmonic oscillator, the pendulum, and the Kepler motion.

coordinate in **Figure 1**, is regarded as "periodic" with period $2\pi h$. In the Kepler case, only the negative-energy trajectories are periodic and a few of them are drawn in **Figure 1**. The single dots represent the equilibrium points in phase space.

The region of phase space where motions are periodic is a set of points (p, q) with the topological structure of $\cup_{u\in U}(\{u\} \times C_u)$, where u is a coordinate varying in an open interval U (e.g., the set of values of the energy), and C_u is a closed curve whose points (p, q) are identified by a coordinate (e.g., by the time necessary for an arbitrarily fixed datum with the same energy to evolve into (p, q)).

In the above cases, [24], if the "radial" coordinate is chosen to be the energy the set U is the interval $(0, +\infty)$ for the harmonic oscillator, $(0, 2mg)$ or $(2mg, +\infty)$ for the pendulum, and $(-\frac{1}{2}mk^2/G^2, 0)$ in the Kepler case. The fixed datum for the reference motion can be taken, in all cases, to be of the form $(0, q_0)$ with the time coordinate t_0 given by [23].

It is remarkable that the energy–time coordinates are canonical coordinates: for instance, in the vicinity of (p_0, q_0) and if $p_0 > 0$, this can be seen by setting

$$S(q, E) = \int_{q_0}^{q} \sqrt{2m(E - V(x))}\mathrm{d}x \qquad [25]$$

and checking that $p = \partial_q S(q, E)$, $t = \partial_E S(q, E)$ are identities if (p, q) and (E, t) are coordinates for the same point so that the criterion expressed by [20] applies.

It is convenient to standardize the coordinates by replacing the time variable by an angle $\alpha = (2\pi/T(E))t$; and instead of the energy any invertible function of it can be used.

It is natural to look for a coordinate $A = A(E)$ such that the map $(p, q) \longleftrightarrow (A, \alpha)$ is a canonical map: this is easily done as the function

$$\hat{S}(q, A) = \int_{q_0}^{q} \sqrt{2m(E(A) - V(x))}\,\mathrm{d}x \qquad [26]$$

generates (locally) the correspondence between $p = \sqrt{2m(E(A) - V(q))}$ and

$$\alpha = E'(A) \int_0^q \frac{\mathrm{d}x}{\sqrt{2m^{-1}(E(A) - V(x))}}$$

Therefore, by the criterion [20], if

$$E'(A) = \frac{2\pi}{T(E(A))}$$

i.e., if $A'(E) = T(E)/2\pi$, the coordinates (A, α) will be canonical coordinates. Hence, by [22], $A(E)$ can be taken as

$$A = \frac{1}{2\pi} 2 \int_{q_-(E)}^{q_+(E)} \sqrt{2m(E - V(q))}\mathrm{d}q$$
$$\equiv \frac{1}{2\pi} \oint p\,\mathrm{d}q \qquad [27]$$

where the last integral is extended to the closed curve of energy E; see **Figure 1**. The *action–angle coordinates* (A, α) are defined in open regions of phase space covered by periodic motions: in action–angle coordinates such regions have the form $W = J \times \mathrm{T}$ of a product of an open interval J and a one-dimensional "torus" $\mathrm{T} = [0, 2\pi]$ (i.e., a unit circle).

For details, the reader is again referred to Landau and Lifshitz (1976), Arnol'd (1989), and Gallavotti (1983).

Quasiperiodicity and Integrability

A Hamiltonian is called *integrable* in an open region $W \subset T^*(M)$ of phase space if

1. there is an analytic and nonsingular (i.e., with nonzero Jacobian) change of coordinates $(\boldsymbol{p}, \boldsymbol{q}) \longleftrightarrow (\boldsymbol{I}, \boldsymbol{\varphi})$ mapping W into a set of the form $\mathcal{I} \times \mathrm{T}^\ell$ with $\mathcal{I} \subset \mathbb{R}^\ell$ (open); and furthermore
2. the flow $t \to S_t(\boldsymbol{p}, \boldsymbol{q})$ on phase space is transformed into $(\boldsymbol{I}, \boldsymbol{\varphi}) \to (\boldsymbol{I}, \boldsymbol{\varphi} + \boldsymbol{\omega}(\boldsymbol{I})t)$ where $\boldsymbol{\omega}(\boldsymbol{I})$ is a smooth function on $\mathcal{I}$.

This means that, in suitable coordinates, which can be called "integrating coordinates," the system appears as a set of ℓ points with coordinates $\boldsymbol{\varphi} = (\varphi_1, \ldots, \varphi_\ell)$ moving on a unit circle at angular velocities $\boldsymbol{\omega}(\boldsymbol{I}) = (\omega_1(\boldsymbol{I}), \ldots, \omega_\ell(\boldsymbol{I}))$ depending on the actions of the initial data.

A system integrable in a region W which, in integrating coordinates $\boldsymbol{I}, \boldsymbol{\varphi}$, has the form $\mathcal{I} \times \mathrm{T}^\ell$ is said to be *anisochronous* if $\det \partial_{\boldsymbol{I}} \boldsymbol{\omega}(\boldsymbol{I}) \neq 0$. It is said to be isochronous if $\boldsymbol{\omega}(\boldsymbol{I}) \equiv \boldsymbol{\omega}$ is independent of $\boldsymbol{I}$. The motions of integrable systems are called *quasiperiodic* with frequency spectrum $\boldsymbol{\omega}(\boldsymbol{I})$, or with *frequencies* $\boldsymbol{\omega}(\boldsymbol{I})/2\pi$, in the coordinates $(\boldsymbol{I}, \boldsymbol{\varphi})$.

Clearly, an integrable system admits ℓ independent constants of motion, the $\boldsymbol{I} = (I_1, \ldots, I_\ell)$, and, for each

choice of I, the other coordinates vary on a "standard" ℓ-dimensional torus $\mathbb{T}^\ell$: hence, it is possible to say that a phase space region of integrability is *foliated* into ℓ-dimensional invariant tori $\mathcal{T}(I)$ parametrized by the values of the constants of motion $I \in \mathcal{I}$.

If an integrable system is anisochronous then it is *canonically integrable*: that is, it is possible to define on W a canonical change of coordinates $(p, q) = C(A, \alpha)$ mapping W onto $J \times \mathbb{T}^\ell$ and such that $\mathcal{H}(C(A, \alpha)) = h(A)$ for a suitable h. Then, if $\omega(A) \stackrel{\text{def}}{=} \partial_A h(A)$, the equations of motion become

$$\dot{A} = 0, \qquad \dot{\alpha} = \omega(A) \qquad [28]$$

Given a system (I, φ) of coordinates integrating an anisochronous system the construction of action–angle coordinates can be performed, in principle, via a classical procedure (under a few extra assumptions).

Let $\gamma_1, \ldots, \gamma_\ell$ be ℓ topologically independent circles on $\mathbb{T}^\ell$, for definiteness let $\gamma_i(I) = \{\varphi \mid \varphi_1 = \varphi_2 = \cdots = \varphi_{i-1} = \varphi_{i+1} = \cdots = 0,\ \varphi_i \in [0, 2\pi]\}$, and set

$$A_i(I) = \frac{1}{2\pi} \oint_{\gamma_i(I)} p \cdot \mathrm{d}q \qquad [29]$$

If the map $I \longleftrightarrow A(I)$ is analytically invertible as $I = I(A)$, the function

$$S(A, \varphi) = (\lambda) \int_0^\varphi p \cdot \mathrm{d}q \qquad [30]$$

is well defined if the integral is over any path λ joining the points $(p(I(A), 0), q(I(A), 0))$ and $(p(I(A), \varphi)), q(I(A), \varphi)$ and lying on the torus parametrized by $I(A)$.

The key remark in the proof that [30] really defines a function of the only variables A, φ is that anisochrony implies the vanishing of the Poisson brackets (cf. [18]): $\{I_i, I_j\} = 0$ (hence also $\{A_i, A_j\} \equiv \sum_{h,k} \partial_{I_k} A_i\, \partial_{I_h} A_j \{I_k, I_h\} = 0$). And the property $\{I_i, I_j\} = 0$ can be checked to be precisely the integrability condition for the differential form $p \cdot \mathrm{d}q$ restricted to the surface obtained by varying q while p is constrained so that (p, q) stays on the surface $I = \text{constant}$, i.e., on the invariant torus of the points with fixed I.

The latter property is necessary and sufficient in order that the function $S(A, \varphi)$ be well defined (i.e., be independent on the integration path λ) up to an additive quantity of the form $\sum_i 2\pi n_i A_i$ with $n = (n_1, \ldots, n_\ell)$ integers.

Then the action–angle variables are defined by the canonical change of coordinates with $S(A, \varphi)$ as generating function, i.e., by setting

$$\alpha_i = \partial_{A_i} S(A, \varphi), \qquad I_i = \partial_{\varphi_i} S(A, \varphi) \qquad [31]$$

and, since the computation of $S(A, \varphi)$ is "reduced to integrations" which can be regarded as a natural extension of the quadratures discussed in the one-dimensional cases, such systems are also called *integrable by quadratures*. The just-described construction is a version of the more general *Arnol'd–Liouville theorem*.

In practice, however, the actual evaluation of the integrals in [29], [30] can be difficult: its analysis in various cases (even as "elementary" as the pendulum) has in fact led to key progress in various domains, for example, in the theory of special functions and in group theory.

In general, any surface on phase space on which the restriction of the differential form $p \cdot \mathrm{d}q$ is locally integrable is called a *Lagrangian manifold*: hence the invariant tori of an anisochronous integrable system are Lagrangian manifolds.

If an integrable system is anisochronous, it cannot admit more than ℓ independent constants of motion; furthermore, it does not admit invariant tori of dimension $> \ell$. Hence ℓ-dimensional invariant tori are called maximal.

Of course, invariant tori of dimension $< \ell$ can also exist: this happens when the variables I are such that the frequencies $\omega(I)$ admit nontrivial rational relations; i.e., there is an integer components vector $\nu \in \mathbb{Z}^\ell$, $\nu = (\nu_1, \ldots, \nu_\ell) \neq 0$ such that

$$\omega(I) \cdot \nu = \sum_i \omega_i(I) \nu_i = 0 \qquad [32]$$

in this case, the invariant torus $\mathcal{T}(I)$ is called *resonant*. If the system is anisochronous then $\det \partial_I \omega(I) \neq 0$ and, therefore, the resonant tori are associated with values of the constants of motion I which form a set of measure zero in the space $\mathcal{I}$ but which is not empty and dense.

Examples of isochronous systems are the systems of harmonic oscillators, i.e., systems with Hamiltonian

$$\sum_{i=1}^{\ell} \frac{1}{2m_i} p_i^2 + \frac{1}{2} \sum_{i,j}^{1,\ell} c_{ij} q_i q_j$$

where the matrix v is a positive-definite matrix. This is an isochronous system with frequencies $\omega = (\omega_1, \ldots, \omega_\ell)$ whose squares are the eigenvalues of the matrix $m_i^{-1/2} c_{ij} m_j^{-1/2}$. It is integrable in the region W of the data $x = (p, q) \in \mathbb{R}^{2\ell}$ such that, setting

$$A_\beta = \frac{1}{2\omega_\beta} \left(\left(\sum_{i=1}^{\ell} \frac{v_{\beta,i} p_i}{\sqrt{m_i}} \right)^2 + \omega_\beta^2 \left(\sum_{i=1}^{\ell} \frac{v_{\beta,i} q_i}{\sqrt{m_i^{-1}}} \right)^2 \right)$$

for all eigenvectors v_β, $\beta = 1, \ldots, \ell$, of the above matrix, the vectors A have all components > 0.

Even though this system is isochronous, it nevertheless admits a system of canonical action–angle coordinates in which the Hamiltonian takes the simplest form

$$h(\boldsymbol{A}) = \sum_{\beta=1}^{\ell} \omega_\beta A_\beta \equiv \boldsymbol{\omega} \cdot \boldsymbol{A} \qquad [33]$$

with

$$\alpha_\beta = -\arctan\left(\frac{\sum_{i=1}^{\ell} \frac{v_{\beta,i} p_i}{\sqrt{m_i}}}{\sum_{i=1}^{\ell} \sqrt{m_i}\omega_\beta v_{\beta,i} q_i} \right)$$

as conjugate angles.

An example of anisochronous system is the *free rotators* or *free wheels*: i.e., ℓ noninteracting points on a circle of radius R or ℓ noninteracting homogeneous coaxial wheels of radius R. If $J_i = m_i R^2$ or, respectively, $J_i = (1/2) m_i R^2$ are the inertia moments and if the positions are determined by ℓ angles $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)$, the angular velocities are constants related to the angular momenta $\boldsymbol{A} = (A_1, \ldots, A_\ell)$ by $\omega_i = A_i / J_i$. The Hamiltonian and the spectrum are

$$h(\boldsymbol{A}) = \sum_{i=1}^{\ell} \frac{1}{2J_i} A_i^2, \qquad \boldsymbol{\omega}(\boldsymbol{A}) = \left(\frac{1}{J_i} A_i \right)_{i=1,\ldots,\ell} \qquad [34]$$

For further details see Landau and Lifshitz (1976), Gallavotti (1983), Arnol'd (1989), and Fassò (1998).

Multidimensional Quadratures: Central Motion

Several important mechanical systems with more than one degree of freedom are integrable by canonical quadratures in vast regions of phase space. This is checked by showing that there is a foliation into invariant tori $\mathcal{T}(\boldsymbol{I})$ of dimension equal to the number of degrees of freedom (ℓ) parametrized by ℓ constants of motion $\boldsymbol{I}$ in involution, i.e., such that $\{I_i, I_j\} = 0$. One then performs, if possible, the construction of the action–angle variables by the quadratures discussed in the previous section.

The above procedure is well illustrated by the theory of the planar motion of a unit mass attracted by a coplanar center of force: the Lagrangian is, in polar coordinates (ρ, θ),

$$\mathcal{L} = \frac{m}{2}(\dot{\rho}^2 + \rho^2 \dot{\theta}^2) - V(\rho)$$

The planarity of the motion is not a strong restriction as central motion always takes place on a plane.

Hence, the equations of motion are

$$\frac{\mathrm{d}}{\mathrm{d}t} m\rho^2 \dot{\theta} = 0$$

i.e., $m\rho^2\dot{\theta} = G$ is a constant of motion (it is the angular momentum), and

$$\begin{aligned} \ddot{\rho} &= -\partial_\rho V(\rho) + \partial_\rho \frac{m}{2} \rho^2 \dot{\theta}^2 \\ &= -\partial_\rho V(\rho) + \frac{G^2}{m\rho^3} \\ &\stackrel{\text{def}}{=} -\partial_\rho V_G(\rho) \end{aligned}$$

Then the energy conservation yields a second constant of motion E,

$$\begin{aligned} &\frac{m}{2}\dot{\rho}^2 + \frac{1}{2}\frac{G^2}{m\rho^2} + V(\rho) = E \\ &\quad = \frac{1}{2m} p_\rho^2 + \frac{1}{2m}\frac{p_\theta^2}{\rho^2} + V(\rho) \end{aligned} \qquad [35]$$

The right-hand side (rhs) is the Hamiltonian for the system, derived from $\mathcal{L}$, if p_ρ, p_θ denote conjugate momenta of ρ, θ: $p_\rho = m\dot{\rho}$ and $p_\theta = m\rho^2\dot{\theta}$ (note that $p_\theta = G$).

Suppose $\rho^2 V(\rho) \underset{\rho \to 0}{\longrightarrow} 0$: then the singularity at the origin cannot be reached by any motion starting with $\rho > 0$ if $G > 0$. Assume also that the function

$$V_G(\rho) \stackrel{\text{def}}{=} \frac{1}{2}\frac{G^2}{m\rho^2} + V(\rho)$$

has only one minimum $E_0(G)$, no maximum and no horizontal inflection, and tends to a limit $E_\infty(G) \leq \infty$ when $\rho \to \infty$. Then the system is integrable in the domain $W = \{(\boldsymbol{p}, \boldsymbol{q}) \mid E_0(G) < E < E_\infty(G), G \neq 0\}$.

This is checked by introducing a "standard" periodic solution $t \to R(t)$ of $m\ddot{\rho} = -\partial_\rho V_G(\rho)$ with energy $E_0(G) < E < E_\infty(G)$ and initial data $\rho = \rho_{E,-}(G)$, $\dot{\rho} = 0$ at time $t = 0$, where $\rho_{E,\pm}(G)$ are the two solutions of $V_G(\rho) = E$, see the section "Quadratures": this is a periodic analytic function of t with period

$$T(E, G) = 2\int_{\rho_{E,-}(G)}^{\rho_{E,+}(G)} \frac{\mathrm{d}x}{\sqrt{(2/m)(E - V_G(x))}}$$

The function $R(t)$ is given, for $0 \leq t \leq \frac{1}{2}T(E, G)$ or for $\frac{1}{2}T(E, G) \leq t \leq T(E, G)$, by the quadratures

$$t = \int_{\rho_{E,-}(G)}^{R(t)} \frac{\mathrm{d}x}{\sqrt{(2/m)(E - V_G(x))}} \qquad [36a]$$

or

$$t = \frac{T(E, G)}{2} - \int_{\rho_{E,+}(G)}^{R(t)} \frac{\mathrm{d}x}{\sqrt{(2/m)(E - V_G(x))}} \qquad [36b]$$

respectively. The analytic regularity of $R(t)$ follows from the general existence, uniqueness, and regularity theorems applied to the differential equation for $\ddot{\rho}$.

Given an initial datum $\dot{\rho}_0, \rho_0, \dot{\theta}_0, \theta_0$ with energy E and angular momentum G, define t_0 to be the time such that $R(t_0) = \rho_0, \dot{R}(t_0) = \dot{\rho}_0$: then $\rho(t) \equiv R(t + t_0)$ and $\theta(t)$ can be computed as

$$\theta(t) = \theta_0 + \int_0^t \frac{G}{mR(t' + t_0)^2} \mathrm{d}t'$$

a second quadrature. Therefore, we can use as coordinates for the motion E, G, t_0, which determine $\dot{\rho}_0, \rho_0, \dot{\theta}_0$ and a fourth coordinate that determines θ_0 which could be θ_0 itself but which is conveniently determined, via the second quadrature, as follows.

The function $Gm^{-1}R(t)^{-2}$ is periodic with period $T(E, G)$; hence it can be expressed in a Fourier series

$$\chi_0(E, G) + \sum_{k \neq 0} \chi_k(E, G) \exp\left(\frac{2\pi}{T(E, G)} itk\right)$$

the quadrature for $\theta(t)$ can be performed by integrating the series terms. Setting

$$\bar{\theta}(t_0) \stackrel{\text{def}}{=} \frac{T(E, G)}{2\pi} \sum_{k \neq 0} \frac{\chi_k(E, G)}{k} \exp\left(\frac{2\pi}{T(E, G)} it_0 k\right)$$

and $\varphi_1(0) = \theta_0 - \bar{\theta}(t_0)$, the expression

$$\theta(t) = \theta_0 + \int_0^t \frac{G}{mR(t' + t_0)^2} \mathrm{d}t'$$

becomes

$$\varphi_1(t) = \varphi_1(0) + \chi_0(E, G)\, t \qquad [37]$$

Hence the system is integrable and the spectrum is $\boldsymbol{\omega}(E, G) = (\omega_0(E, G), \omega_1(E, G)) \equiv (\omega_0, \omega_1)$ with

$$\omega_0 \stackrel{\text{def}}{=} \frac{2\pi}{T(E, G)} \quad \text{and} \quad \omega_1 \stackrel{\text{def}}{=} \chi_0(E, G)$$

while $I = (E, G)$ are constants of motion and the angles $\boldsymbol{\varphi} = (\varphi_0, \varphi_1)$ can be taken as

$$\varphi_0 \stackrel{\text{def}}{=} \omega_0 t_0, \qquad \varphi_1 \stackrel{\text{def}}{=} \theta_0 - \bar{\theta}(t_0)$$

At E, G fixed, the motion takes place on a two-dimensional torus $\mathcal{T}(E, G)$ with φ_0, φ_1 as angles.

In the anisochronous cases, i.e., when $\det \partial_{E,G} \boldsymbol{\omega}(E, G) \neq 0$, canonical action–angle variables conjugated to $(p_\rho, \rho, p_\theta, \theta)$ can be constructed via [29], [30] by using two cycles γ_1, γ_2 on the torus $\mathcal{T}(E, G)$. It is convenient to choose

1. γ_1 as the cycle consisting of the points $\rho = x, \theta = 0$ whose first half (where $p_\rho \geq 0$) consists in the set $\rho_{E,-}(G) \leq x \leq \rho_{E,+}(G), p_\rho = \sqrt{2m(E - V_G(x))}$ and $\mathrm{d}\theta = 0$; and
2. γ_2 as the cycle $\rho = \text{const}, \theta \in [0, 2\pi]$ on which $\mathrm{d}\rho = 0$ and $p_\theta = G$ obtaining

$$A_1 = \frac{2}{2\pi} \int_{\rho_{E,-}(G)}^{\rho_{E,+}(G)} \sqrt{2m(E - V_G(x))}\mathrm{d}x, \qquad [38]$$
$$A_2 = G$$

According to the general theory (cf. the previous section) a generating function for the canonical change of coordinates from $(p_\rho, \rho, p_\theta, \theta)$ to action–angle variables is (if, to fix ideas, $p_\rho > 0$)

$$S(A_1, A_2, \rho, \theta) = G\theta + \int_{\rho_{E,-}}^{\rho} \sqrt{2m(E - V_G(x))}\mathrm{d}x \qquad [39]$$

In terms of the above ω_0, χ_0 the Jacobian matrix $\partial(E, G)/\partial(A_1, A_2)$ is computed from [38], [39] to be $\begin{pmatrix} \omega_0 & \chi_0 \\ 0 & 1 \end{pmatrix}$. It follows that $\partial_E S = t, \partial_G S = \theta - \bar{\theta}(t) - \chi_0{}^t$ so that, see [31],

$$\alpha_1 \stackrel{\text{def}}{=} \partial_{A_1} S = \omega_0 t, \qquad \alpha_2 \stackrel{\text{def}}{=} \partial_{A_2} S = \theta - \bar{\theta}(t) \qquad [40]$$

and $(A_1, \alpha_1), (A_2, \alpha_2)$ are the action–angle pairs.

For more details, see Landau and Lifshitz (1976) and Gallavotti (1983).

Newtonian Potential and Kepler's Laws

The anisochrony property, that is, $\det \partial(\omega_0, \chi_0)/\partial(A_1, A_2) \neq 0$ or, equivalently, $\det \partial(\omega_0, \chi_0)/\partial(E, G) \neq 0$, is not satisfied in the important cases of the harmonic potential and the Newtonian potential. Anisochrony being only a sufficient condition for canonical integrability it is still possible (and true) that, nevertheless, in both cases the canonical transformation generated by [39] integrates the system. This is expected since the two potentials are limiting cases of anisochronous ones (e.g., $|q|^{2+\varepsilon}$ and $|q|^{-1-\varepsilon}$ with $\varepsilon \to 0$).

The Newtonian potential

$$\mathcal{H}(p, q) = \frac{1}{2m} p^2 - \frac{km}{|q|}$$

is integrable in the region $G \neq 0$, $E_0(G) = -k^2m^3/2G^2 < E < 0$, $|G| < \sqrt{k^2m^3/(-2E)}$. Proceeding as in the last section, one finds integrating coordinates and that the integrable motions develop on ellipses with one focus on the center of attraction S so that motions are periodic, hence not anisochronous: nevertheless, the construction of the canonical coordinates via [29]–[31] (hence [39]) works and leads to canonical coordinates $(L', \lambda', G', \gamma')$. To obtain action–angle variables with a simple

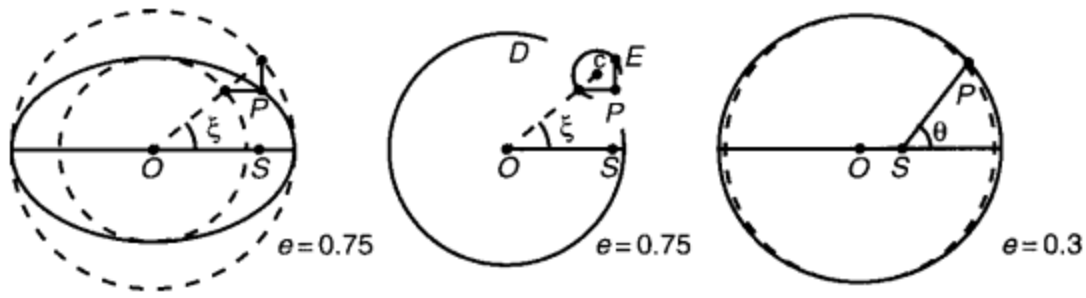

Figure 2 Eccentric and true anomalies of P, which moves on a small circle E centered at a point c moving on the circle D located half-way between the two concentric circles containing the Keplerian ellipse: the anomaly of c with respect to the axis OS is ξ. The circle D is *eccentric* with respect to S and therefore ξ is, even today, called eccentric anomaly, whereas the circle D is, in ancient terminology, the *deferent* circle (eccentric circles were introduced in astronomy by Ptolemy). The small circle E on which the point P moves is, in ancient terminology, an *epicycle*. The deferent and the epicyclical motions are synchronous (i.e., they have the same period); Kepler discovered that his key *a priori* hypothesis of inverse proportionality between angular velocity on the deferent and distance between P and S (i.e., $\rho\dot{\xi} = \text{constant}$) implied both synchrony and elliptical shape of the orbit, with focus in S. The latter law is equivalent to $\rho^2\dot{\theta} = \text{constant}$ (because of the identity $a\dot{\xi} = \rho\dot{\theta}$). Small eccentricity ellipses can hardly be distinguished from circles.

interpretation, it is convenient to perform on the variables $(L', \lambda', G', \gamma')$ (constructed by following the procedure just indicated) a further trivial canonical transformation by setting $L = L' + G'$, $G = G'$, $\lambda = \lambda'$, $\gamma = \gamma' - \lambda'$; then

1. λ (average anomaly) is the time necessary for the point P to move from the pericenter to its actual position, in units of the period, times 2π;
2. L (action) is essentially the energy $E = -k^2m^3/2L^2$;
3. G (angular momentum);
4. γ (axis longitude), is the angle between a fixed axis and the major axis of the ellipse oriented from the center of the ellipse O to the center of attraction S.

The eccentricity of the ellipse is e such that $G = \pm L\sqrt{1-e^2}$. The ellipse equation is $\rho = a(1 - e\cos\xi)$, where ξ is the eccentric anomaly (see **Figure 2**), $a = L^2/km^2$ is the major semiaxis, and ρ is the distance to the center of attraction S.

Finally, the relations between eccentric anomaly ξ, average anomaly λ, true anomaly θ (the latter is the polar angle), and SP distance ρ are given by the Kepler equations

$$\begin{aligned} &\lambda = \xi - e\sin\xi \\ &(1 - e\cos\xi)(1 + e\cos\theta) = 1 - e^2 \\ &\lambda = (1-e^2)^{3/2}\int_0^{\theta} \frac{d\theta'}{(1+e\cos\theta')^2} \\ &\frac{\rho}{a} = \frac{1-e^2}{1+e\cos\theta} \end{aligned} \qquad [41]$$

and the relation between true anomaly and average anomaly can be inverted in the form

$$\begin{aligned} &\xi = \lambda + g_\lambda \\ &\theta = \lambda + f_\lambda \;\Rightarrow\; \frac{\rho}{a} = \frac{1-e^2}{1+e\cos(\lambda + f_\lambda)} \end{aligned} \qquad [42]$$

where $g_\lambda = g(e\sin\lambda, e\cos\lambda)$, $f_\lambda = f(e\sin\lambda, e\cos\lambda)$, and $g(x,y), f(x,y)$ are suitable functions analytic for $|x|, |y| < 1$. Furthermore, $g(x,y) = x(1 + y + \cdots)$, $f(x,y) = 2x(1 + \frac{5}{4}y + \cdots)$ and the ellipses denote terms of degree 2 or higher in x, y, containing only even powers of x.

For more details, the reader is referred to Landau and Lifshitz (1976) and Gallavotti (1983).

Rigid Body

Another fundamental integrable system is the rigid body in the absence of gravity and with a fixed point O. It can be naturally described in terms of the Euler angles $\theta_0, \varphi_0, \psi_0$ (see **Figure 3**) and their derivatives $\dot{\theta}_0, \dot{\varphi}_0, \dot{\psi}_0$.

Let I_1, I_2, I_3 be the three *principal inertia moments* of the body along the three principal axes with unit vectors $\boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3$. The inertia moments and the principal axes are the eigenvalues and the associated unit eigenvectors of the 3×3 inertia matrix $\mathcal{I}$, which is defined by $\mathcal{I}_{hk} = \sum_{i=1}^{n} m_i(\boldsymbol{x}_i)_h(\boldsymbol{x}_i)_k$, where $h, k = 1, 2, 3$ and $\boldsymbol{x}_i$ is the position of the ith particle in a reference frame with origin at O and in which



Figure 3 The *Euler angles* of the comoving frame $\boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3$ with respect to a fixed frame $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$. The direction $\boldsymbol{n}$ is the "node line, intersection between the planes $\boldsymbol{x}, \boldsymbol{y}$ and $\boldsymbol{i}_1, \boldsymbol{i}_2$.

all particles are at rest: this *comoving frame* exists as a consequence of the rigidity constraint. The principal axes form a coordinate system which is comoving as well: that is, in the frame $(O; \boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3)$ as well, the particles are at rest.

The Lagrangian is simply the kinetic energy: we imagine the rigidity constraint to be ideal (e.g., as realized by internal central forces in the limit of infinite rigidity, as mentioned in the section "Lagrange and Hamilton forms of equations of motion"). The *angular velocity* of the rigid motion is defined by

$$\boldsymbol{\omega} = \dot{\theta}_0 \boldsymbol{n} + \dot{\varphi}_0 \boldsymbol{z} + \dot{\psi}_0 \boldsymbol{i}_3 \qquad [43]$$

expressing that a generic infinitesimal motion must consist of a variation of the three Euler angles and, therefore, it has to be a rotation of speeds $\dot{\theta}_0, \dot{\varphi}_0, \dot{\psi}_0$ around the axes $\boldsymbol{n}, \boldsymbol{z}, \boldsymbol{i}_3$ as shown in **Figure 3**.

Let $(\omega_1, \omega_2, \omega_3)$ be the components of $\boldsymbol{\omega}$ along the principal axes $\boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3$: for brevity, the latter axes will often be called **1, 2, 3**. Then the angular momentum $\boldsymbol{M}$, with respect to the pivot point O, and the kinetic energy K can be checked to be

$$\begin{aligned} \boldsymbol{M} &= I_1\omega_1\boldsymbol{i}_1 + I_2\omega_2\boldsymbol{i}_2 + I_3\omega_3\boldsymbol{i}_3 \\ K &= \frac{1}{2}(I_1\omega_1^2 + I_2\omega_2^2 + I_2\omega_3^2) \end{aligned} \qquad [44]$$

and are constants of motion. From **Figure 3** it follows that $\omega_1 = \dot{\theta}_0 \cos\psi_0 + \dot{\varphi}_0 \sin\theta_0 \sin\psi_0$, $\omega_2 = -\dot{\theta}_0 \sin\psi_0 + \dot{\varphi}_0 \sin\theta_0 \cos\psi_0$ and $\omega_3 = \dot{\varphi}_0 \cos\theta_0 + \dot{\psi}_0$, so that the Lagrangian, uninspiring at first, is

$$\begin{aligned} \mathcal{L} \stackrel{\text{def}}{=} & \frac{1}{2} I_1 (\dot{\theta}_0 \cos\psi_0 + \dot{\varphi}_0 \sin\theta_0 \sin\psi_0)^2 \\ & + \frac{1}{2} I_2 (-\dot{\theta}_0 \sin\psi_0 + \dot{\varphi}_0 \sin\theta_0 \cos\psi_0)^2 \\ & + \frac{1}{2} I_3 (\dot{\varphi}_0 \cos\theta_0 + \dot{\psi}_0)^2 \end{aligned} \qquad [45]$$

Angular momentum conservation does not imply that the components ω_j are constants because $\boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3$ also change with time according to

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{i}_j = \boldsymbol{\omega} \wedge \boldsymbol{i}_j, \quad j = 1, 2, 3$$

Hence, $\dot{\boldsymbol{M}} = 0$ becomes, by the first of [44] and denoting $I\boldsymbol{\omega} = (I_1\omega_1, I_2\omega_2, I_3\omega_3)$, the *Euler equations* $I\dot{\boldsymbol{\omega}} + \boldsymbol{\omega} \wedge I\boldsymbol{\omega} = 0$, or

$$\begin{aligned} I_1\dot{\omega}_1 &= (I_2 - I_3)\omega_2\omega_3 \\ I_2\dot{\omega}_2 &= (I_3 - I_1)\omega_3\omega_1 \\ I_3\dot{\omega}_3 &= (I_1 - I_2)\omega_1\omega_2 \end{aligned} \qquad [46]$$

which can be considered together with the conserved quantities [44].

Since angular momentum is conserved, it is convenient to introduce the *laboratory frame* $(O; \boldsymbol{x}_0, \boldsymbol{y}_0, \boldsymbol{z}_0)$ with fixed axes $\boldsymbol{x}_0, \boldsymbol{y}_0, \boldsymbol{z}_0$ and (see **Figure 4**):

1. $(O; \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$, the *momentum frame* with fixed axes, but with z-axis oriented as $\boldsymbol{M}$, and x-axis coinciding with the node (i.e., the intersection) of the x_0–y_0 plane and the x–y plane (orthogonal to $\boldsymbol{M}$). Therefore, $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$ is determined by the two Euler angles ζ, γ of $(O; \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ in $(O; \boldsymbol{x}_0, \boldsymbol{y}_0, \boldsymbol{z}_0)$;
2. $(O; \mathbf{1}, \mathbf{2}, \mathbf{3})$, the comoving frame, that is, the frame fixed with the body, and with unit vectors $\boldsymbol{i}_1, \boldsymbol{i}_2, \boldsymbol{i}_3$ parallel to the principal axes of the body. The frame is determined by three Euler angles $\theta_0, \varphi_0, \psi_0$;
3. the Euler angles of $(O; \mathbf{1}, \mathbf{2}, \mathbf{3})$ with respect to $(O; \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$, which are denoted θ, φ, ψ;
4. G, the total angular momentum: $G^2 = \sum_j I_j^2 \omega_j^2$;
5. M_3, the angular momentum along the z_0 axis; $M_3 = G\cos\zeta$; and
6. L, the projection of $\boldsymbol{M}$ on the axis **3**, $L = G\cos\theta$.

The quantities $G, M_3, L, \varphi, \gamma, \psi$ determine $\theta_0, \varphi_0, \psi_0$ and $\dot{\theta}_0, \dot{\varphi}_0, \dot{\psi}_0$, or the $p_{\theta_0}, p_{\varphi_0}, p_{\psi_0}$ variables conjugated to $\theta_0, \varphi_0, \psi_0$ as shown by the following comment.

Considering **Figure 4**, the angles ζ, γ determine location, in the fixed frame $(O; \boldsymbol{x}_0, \boldsymbol{y}_0, \boldsymbol{z}_0)$ of the direction of $\boldsymbol{M}$ and the node line $\boldsymbol{m}$, which are, respectively, the z-axis and the x-axis of the fixed frame associated with the angular momentum; the angles θ, φ, ψ then determine the position of the comoving frame with respect to the fixed frame $(O; \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$, hence its position with respect to $(O; \boldsymbol{x}_0, \boldsymbol{y}_0, \boldsymbol{z}_0)$, that is, $(\theta_0, \varphi_0, \psi_0)$. From this and G, it is possible to determine $\boldsymbol{\omega}$ because

$$\begin{aligned} \cos\theta &= \frac{I_3\omega_3}{G}, \qquad \tan\psi = \frac{I_2\omega_2}{I_1\omega_1} \\ \omega_2^2 &= I_2^{-2}(G^2 - I_1^2\omega_1^2 - I_3^2\omega_3^2) \end{aligned} \qquad [47]$$

and, from [43], $\dot{\theta}_0, \dot{\varphi}_0, \dot{\psi}_0$ are determined.

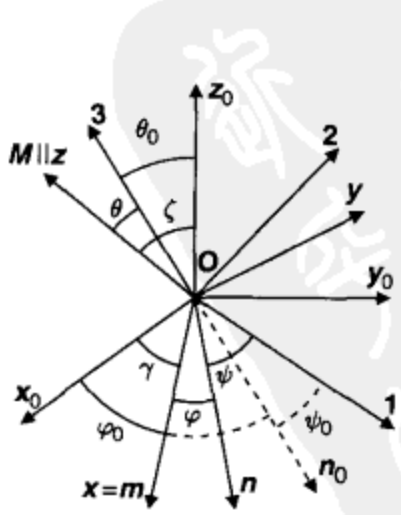

Figure 4 The laboratory frame, the angular momentum frame, and the comoving frame (and the Deprit angles).

The Lagrangian [45] gives immediately (after expressing $\boldsymbol{\omega}$, i.e., $\boldsymbol{n}, \boldsymbol{z}, \boldsymbol{i}_3$, in terms of the Euler angles $\theta_0, \varphi_0, \psi_0$) an expression for the variables $p_{\theta_0}, p_{\varphi_0}, p_{\psi_0}$ conjugated to $\theta_0, \varphi_0, \psi_0$:

$$p_{\theta_0} = \boldsymbol{M} \cdot \boldsymbol{n}_0, \quad p_{\varphi_0} = \boldsymbol{M} \cdot \boldsymbol{z}_0, \quad p_{\psi_0} = \boldsymbol{M} \cdot \boldsymbol{i}_3 \qquad [48]$$

and, in principle, we could proceed to compute the Hamiltonian.

However, the computation can be avoided because of the very remarkable property (Deprit), which can be checked with some patience, making use of [48] and of elementary spherical trigonometry identities,

$$\begin{aligned} M_3\,\mathrm{d}\gamma + G\,\mathrm{d}\varphi + L\,\mathrm{d}\psi \\ = p_{\varphi_0}\,\mathrm{d}\varphi_0 + p_{\psi_0}\,\mathrm{d}\psi_0 + p_{\theta_0}\,\mathrm{d}\theta_0 \end{aligned} \qquad [49]$$

which means that the map $((M_3, \gamma), (L, \psi), (G, \varphi)) \longleftrightarrow ((p_{\theta_0}, \theta_0), (p_{\varphi_0}, \varphi_0), (p_{\psi_0}, \psi_0))$ is a canonical map. And in the new coordinates, the kinetic energy, hence the Hamiltonian, takes the form

$$K = \frac{1}{2}\left[\frac{L^2}{I_3} + (G^2 - L^2)\left(\frac{\sin^2\psi}{I_1} + \frac{\cos^2\psi}{I_2}\right)\right] \qquad [50]$$

This again shows that G, M_3 are constants of motion, and the L, ψ variables are determined by a quadrature, because the Hamilton equation for ψ combined with the energy conservation yields

$$\begin{aligned} \dot{\psi} = \pm &\left(\frac{1}{I_3} - \frac{\sin^2\psi}{I_1} - \frac{\cos^2\psi}{I_2}\right) \\ &\times \sqrt{\frac{2E - G^2\left(\frac{\sin^2\psi}{I_1} + \frac{\cos^2\psi}{I_2}\right)}{\frac{1}{I_3} - \frac{\sin^2\psi}{I_1} - \frac{\cos^2\psi}{I_2}}} \end{aligned} \qquad [51]$$

In the integrability region, this motion is periodic with some period $T_L(E, G)$. Once $\psi(t)$ is determined, the Hamilton equation for φ leads to the further quadrature

$$\dot{\varphi} = \left(\frac{\sin^2\psi(t)}{I_1} + \frac{\cos^2\psi(t)}{I_2}\right) G \qquad [52]$$

which determines a second periodic motion with period $T_G(E, G)$. The γ, M_3 are constants and, therefore, the motion takes place on three-dimensional invariant tori $\mathcal{T}_{E,G,M_3}$ in phase space, each of which is "always" foliated into two-dimensional invariant tori parametrized by the angle γ which is constant (by [50], because K is M_3-independent): the latter are in turn foliated by one-dimensional invariant tori, that is, by periodic orbits, with E, G such that the value of $T_L(E, G)/T_G(E, G)$ is rational.

Note that if $I_1 = I_2 = I$, the above analysis is extremely simplified. Furthermore, if gravity g acts on the system the Hamiltonian will simply change by the addition of a potential $-mgz$ if z is the height of the center of mass. Then (see **Figure 4**), if the center of mass of the body is on the axis $\boldsymbol{i}_3$ and $z = h\cos\theta_0$, and h is the distance of the center of mass from O, since $\cos\theta_0 = \cos\theta\cos\zeta - \sin\theta\sin\zeta\cos\varphi$, the Hamiltonian will become $\mathcal{H} = K - mgh\cos\theta_0$ or

$$\begin{aligned} \mathcal{H} = &\frac{G^2}{2I_3} + \frac{G^2 - L^2}{2I} - mgh\left(\frac{M_3 L}{G^2} - \left(1 - \frac{M_3^2}{G^2}\right)^{1/2}\right. \\ &\left.\times\left(1 - \frac{L^2}{G^2}\right)^{1/2}\cos\varphi\right) \end{aligned} \qquad [53]$$

so that, again, the system is integrable by quadratures (with the roles of ψ and φ "interchanged" with respect to the previous case) in suitable regions of phase space. This is called the *Lagrange's gyroscope*.

A less elementary integrable case is when the inertia moments are related as $I_1 = I_2 = 2I_3$ and the center of mass is in the $\boldsymbol{i}_1$–$\boldsymbol{i}_2$ plane (rather than on the $\boldsymbol{i}_3$-axis) and only gravity acts, besides the constraint force on the pivot point O; this is called *Kowalevskaia's gyroscope*.

For more details, see Gallavotti (1983).

Other Quadratures

An interesting classical integrable motion is that of a point mass attracted by two equal-mass centers of gravitational attraction, or a point ideally constrained to move on the surface of a general ellipsoid.

New integrable systems have been discovered quite recently and have generated a wealth of new developments ranging from group theory (as integrable systems are closely related to symmetries) to partial differential equations.

It is convenient to extend the notion of integrability by stating that a system is integrable in a region W of phase space if

1. there is a change of coordinates $(\boldsymbol{p}, \boldsymbol{q}) \in W \longleftrightarrow \{\boldsymbol{A}, \boldsymbol{\alpha}, \boldsymbol{Y}, \boldsymbol{y}\} \in (U \times \mathbb{T}^\ell) \times (V \times \mathbb{R}^m)$ where $U \subset \mathbb{R}^\ell$, $V \subset \mathbb{R}^m$, with $\ell + m \geq 1$, are open sets; and
2. the $\boldsymbol{A}, \boldsymbol{Y}$ are constants of motion while the other coordinates vary "linearly":

$$(\boldsymbol{\alpha}, \boldsymbol{y}) \to (\boldsymbol{\alpha} + \boldsymbol{\omega}(\boldsymbol{A}, \boldsymbol{Y})t,\ \boldsymbol{y} + \boldsymbol{\nu}(\boldsymbol{A}, \boldsymbol{Y})t) \qquad [54]$$

where $\boldsymbol{\omega}(\boldsymbol{A}, \boldsymbol{Y}), \boldsymbol{\nu}(\boldsymbol{A}, \boldsymbol{Y})$ are smooth functions.

In the new sense, the systems studied in the previous sections are integrable in much wider regions (essentially on the entire phase space with the exception of a set of data which lie on lower-dimensional surfaces

forming sets of zero volume). The notion is convenient also because it allows us to say that even the systems of free particles are integrable.

Two very remarkable systems integrable in the new sense are the Hamiltonian systems, respectively called *Toda lattice* (KRUSKAL, ZABUSKY), and *Calogero lattice* (CALOGERO, MOSER); if $(p_i, q_i) \in \mathbb{R}^2$, they are

$$\mathcal{H}_T(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{2m}\sum_{i=1}^{n} p_i^2 + \sum_{i=1}^{n-1} g\, e^{-\kappa(q_{i+1}-q_i)}$$

$$\mathcal{H}_C(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{2m}\sum_{i=1}^{n} p_i^2 + \sum_{i<j}^{n} \frac{g}{(q_i-q_j)^2} + \frac{1}{2}\sum_{i=1}^{n} m\omega^2 q_i^2 \qquad [55]$$

where $m > 0$ and $\kappa, \omega, g \geq 0$. They describe the motion of n interacting particles on a line.

The integration method for the above systems is again to find first the constants of motion and later to look for quadratures, when appropriate. The constants of motion can be found with the method of the *Lax pairs*. One shows that there is a pair of self-adjoint $n \times n$ matrices $M(\boldsymbol{p},\boldsymbol{q}), N(\boldsymbol{p},\boldsymbol{q})$ such that the equations of motion become

$$\frac{\mathrm{d}}{\mathrm{d}t} M(\boldsymbol{p},\boldsymbol{q}) = \mathrm{i}[M(\boldsymbol{p},\boldsymbol{q}), N(\boldsymbol{p},\boldsymbol{q})], \quad \mathrm{i} = \sqrt{-1} \qquad [56]$$

which imply that $M(t) = U(t)M(0)U(t)^{-1}$, with $U(t)$ a unitary matrix. When the equations can be written in the above form, it is clear that the n eigenvalues of the matrix $M(0) = M(\boldsymbol{p}_0, \boldsymbol{q}_0)$ are constants of motion. When appropriate (e.g., in the Calogero lattice case with $\omega > 0$), it is possible to proceed to find canonical action–angle coordinates: a task that is quite difficult due to the arbitrariness of n, but which is possible.

The Lax pairs for the Calogero lattice (with $\omega = 0$, $g = m = 1$) are

$$M_{hh} = p_h, \qquad N_{hh} = 0$$
$$M_{hk} = \frac{\mathrm{i}}{(q_h - q_k)}, \qquad N_{hk} = \frac{1}{(q_h - q_k)^2} \quad h \neq k \qquad [57]$$

while for the Toda lattice (with $m = g = \frac{1}{2}\kappa = 1$) the nonzero matrix elements of M, N are

$$M_{hh} = p_h, \qquad M_{h,h+1} = M_{h+1,h} = e^{-(q_h - q_{h+1})}$$
$$N_{h,h+1} = -N_{h+1,h} = \mathrm{i}\, e^{-(q_h - q_{h+1})} \qquad [58]$$

which are checked by first trying the case $n = 2$.

Another integrable system (SUTHERLAND) is

$$\mathcal{H}_S(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{2m}\sum_{i=k}^{n} p_k^2 + \sum_{h<k}^{n} \frac{g}{\sinh^2(q_h - q_k)} \qquad [59]$$

whose Lax pair is related to that of the Calogero lattice.

By taking suitable limits as $n \to \infty$ and as the other parameters tend to 0 or ∞ at suitable rates, integrability of a few differential equations, among which the *Korteweg–deVries equation* or the nonlinear *Schrödinger equation*, can be derived.

As mentioned in the introductory section, symmetry properties under continuous groups imply existence of constants of motion. Hence, it is natural to think that integrability of a mechanical system reflects enough symmetry to imply the existence of as many constants of motion, independent and in involution, as the number of degrees of freedom, n.

This is in fact always true, and in some respects it is a tautological statement in the anisochronous cases. Integrability in a region W implies existence of canonical action–angle coordinates $(\boldsymbol{A}, \boldsymbol{\alpha})$ (see the section "Quasiperiodicity and integrability") and the Hamiltonian depends solely on the $\boldsymbol{A}$'s: therefore, its restriction to W is invariant with respect to the action of the continuous commutative group $\mathcal{T}^n$ of the translations of the angle variables. The actions can be seen as constants of motion whose existence follows from Noether's theorem, at least in the anisochronous cases in which the Hamiltonian formulation is equivalent to a Lagrangian one.

What is nontrivial is to recognize, prior to realizing integrability, that a system admits this kind of symmetry: in most of the interesting cases, the systems either do not exhibit obvious symmetries or they exhibit symmetries apparently unrelated to the group $\mathcal{T}^n$, which nevertheless imply existence of sufficiently many independent constants of motion as required for integrability. Hence, nontrivial integrable systems possess a "hidden" symmetry under $\mathcal{T}^n$: the rigid body is an example.

However, very often the symmetries of a Hamiltonian H which imply integrability also imply partial isochrony, that is, they imply that the number of independent frequencies is smaller than n (see the section "Quasiperiodicity and integrability"). Even in such cases, often a map exists from the original coordinates $(\boldsymbol{p},\boldsymbol{q})$ to the integrating variables $(\boldsymbol{A},\boldsymbol{\alpha})$ in which $\boldsymbol{A}$ are constants of motion and the $\boldsymbol{\alpha}$ are uniformly rotating angles (some of which are also constant) with spectrum $\boldsymbol{\omega}(\boldsymbol{A})$, which is the gradient $\partial_{\boldsymbol{A}} h(\boldsymbol{A})$ for some function $h(\boldsymbol{A})$ depending only on a few of the $\boldsymbol{A}$ coordinates. However, the map might fail to be canonical. The system is then said to be bi-Hamiltonian: in the sense that one can represent motions in two systems of canonical coordinates, not related by a canonical transformation, and by two Hamiltonian functions H and $H' \equiv h$ which generate the same motions in the respective

coordinates (the latter changes of variables are sometimes called "canonical with respect to the pair H, H'" while the transformations considered in the section "Canonical transformations of phase space coordination" are called completely canonical).

For more details, we refer the reader to Calogero and Degasperis (1982).

Generic Nonintegrability

It is natural to try to prove that a system "close" to an integrable one has motions with properties very close to quasiperiodic. This is indeed the case, but in a rather subtle way. That there is a problem is easily seen in the case of a perturbation of an anisochronous integrable system.

Assume that a system is integrable in a region W of phase space which, in the integrating action–angle variables $(\boldsymbol{A}, \boldsymbol{\alpha})$, has the standard form $U \times \mathbb{T}^\ell$ with a Hamiltonian $h(\boldsymbol{A})$ with gradient $\boldsymbol{\omega}(\boldsymbol{A}) = \partial_{\boldsymbol{A}} h(\boldsymbol{A})$. If the forces are perturbed by a potential which is smooth then the new system will be described, in the same coordinates, by a Hamiltonian like

$$\mathcal{H}_\varepsilon(\boldsymbol{A}, \boldsymbol{\alpha}) = h(\boldsymbol{A}) + \varepsilon f(\boldsymbol{A}, \boldsymbol{\alpha}) \qquad [60]$$

with h, f analytic in the variables $\boldsymbol{A}, \boldsymbol{\alpha}$.

If the system really behaved like the unperturbed one, it ought to have ℓ constants of motion of the form $F_\varepsilon(\boldsymbol{A}, \boldsymbol{\alpha})$ analytic in ε near $\varepsilon = 0$ and uniform, that is, single valued (which is the same as periodic) in the variables $\boldsymbol{\alpha}$. However, the following theorem (POINCARÉ) shows that this is a somewhat unlikely possibility.

Theorem 1 *If the matrix $\partial^2_{\boldsymbol{AA}} h(\boldsymbol{A})$ has rank ≥ 2, the Hamiltonian* [60] "*generically*" (an intuitive notion precised below) *cannot be integrated by a canonical transformation $C_\varepsilon(\boldsymbol{A}, \boldsymbol{\alpha})$ which*

(i) *reduces to the identity as $\varepsilon \to 0$; and*
(ii) *is analytic in ε near $\varepsilon = 0$ and in $(\boldsymbol{A}, \boldsymbol{\alpha}) \in U' \times \mathbb{T}^\ell$, with $U' \subset U$ open.*

Furthermore, no uniform constants of motion $F_\varepsilon(\boldsymbol{A}, \boldsymbol{\alpha})$, defined for ε near 0 and $(\boldsymbol{A}, \boldsymbol{\alpha})$ in an open domain $U' \times \mathbb{T}^\ell$, exist other than the functions of $\mathcal{H}_\varepsilon$ itself.

Integrability in the sense (i), (ii) can be called analytic integrability and it is the strongest (and most naive) sense that can be given to the attribute.

The first part of the theorem, that is, (i), (ii), holds simply because, if integrability was assumed, a generating function of the integrating map would have the form $\boldsymbol{A}' \cdot \boldsymbol{\alpha} + \Phi_\varepsilon(\boldsymbol{A}', \boldsymbol{\alpha})$ with Φ admitting a power series expansion in ε as $\Phi_\varepsilon = \varepsilon\Phi^1 + \varepsilon^2\Phi^2 + \cdots$. Hence, Φ^1 would have to satisfy

$$\boldsymbol{\omega}(\boldsymbol{A}') \cdot \partial_{\boldsymbol{\alpha}} \Phi^1(\boldsymbol{A}', \boldsymbol{\alpha}) + f(\boldsymbol{A}', \boldsymbol{\alpha}) = \bar{f}(\boldsymbol{A}') \qquad [61]$$

where $\bar{f}(\boldsymbol{A}')$ depends only on $\boldsymbol{A}'$ (hence integrating both sides with respect to $\boldsymbol{\alpha}$, it appears that $\bar{f}(\boldsymbol{A}')$ must coincide with the average of $f(\boldsymbol{A}', \boldsymbol{\alpha})$ over $\boldsymbol{\alpha}$).

This implies that the Fourier transform $f_{\boldsymbol{\nu}}(\boldsymbol{A})$, $\boldsymbol{\nu} \in \mathbb{Z}^\ell$, should satisfy

$$f_{\boldsymbol{\nu}}(\boldsymbol{A}') = 0 \qquad \text{if } \boldsymbol{\omega}(\boldsymbol{A}') \cdot \boldsymbol{\nu} = 0, \quad \boldsymbol{\nu} \neq \boldsymbol{0} \qquad [62]$$

which is equivalent to the existence of $\tilde{f}_{\boldsymbol{\nu}}(\boldsymbol{A}')$ such that $f_{\boldsymbol{\nu}}(\boldsymbol{A}) = \boldsymbol{\omega}(\boldsymbol{A}') \cdot \boldsymbol{\nu} \tilde{f}_{\boldsymbol{\nu}}(\boldsymbol{A})$ for $\boldsymbol{\nu} \neq 0$. But since there is no relation between $\boldsymbol{\omega}(\boldsymbol{A})$ and $f(\boldsymbol{A}, \boldsymbol{\alpha})$, this property "generically" will not hold in the sense that as close as wished to an f which satisfies the property [62] there will be another f which does not satisfy it essentially no matter how "closeness" is defined, (e.g., with respect to the metric $||f - g|| = \sum_{\boldsymbol{\nu}} |f_{\boldsymbol{\nu}}(\boldsymbol{A}) - g_{\boldsymbol{\nu}}(\boldsymbol{A})||$). This is so because the rank of $\partial^2_{\boldsymbol{AA}} h(\boldsymbol{A})$ is higher than 1 and $\boldsymbol{\omega}(\boldsymbol{A})$ varies at least on a two-dimensional surface, so that $\boldsymbol{\omega} \cdot \boldsymbol{\nu} = 0$ becomes certainly possible for some $\boldsymbol{\nu} \neq 0$ while $f_{\boldsymbol{\nu}}(\boldsymbol{A})$ in general will not vanish, so that Φ^1, hence Φ_ε, does not exist.

This means that close to a function f there is a function f' which violates [62] for some $\boldsymbol{\nu}$. Of course, this depends on what is meant by "close": however, here essentially any topology introduced on the space of the functions f will make the statement correct. For instance, if the distance between two functions is defined by $\sum_{\boldsymbol{\nu}} \sup_{\boldsymbol{A} \in U} |f_{\boldsymbol{\nu}}(\boldsymbol{A}) - g_{\boldsymbol{\nu}}(\boldsymbol{A})|$ or by $\sup_{\boldsymbol{A}, \boldsymbol{\alpha}} |f(\boldsymbol{A}, \boldsymbol{\alpha}) - g(\boldsymbol{A}, \boldsymbol{\alpha})|$.

The idea behind the last statement of the theorem is in essence the same: consider, for simplicity, the anisochronous case in which the matrix $\partial^2_{\boldsymbol{AA}} h(\boldsymbol{A})$ has maximal rank ℓ, that is, the determinant $\det \partial^2_{\boldsymbol{AA}} h(\boldsymbol{A})$ does not vanish. Anisochrony implies that $\boldsymbol{\omega}(\boldsymbol{A}) \cdot \boldsymbol{\nu} \neq 0$ for all $\boldsymbol{\nu} \neq 0$ and $\boldsymbol{A}$ on a dense set, and this property will be used repeatedly in the following analysis.

Let $B(\varepsilon, \boldsymbol{A}, \boldsymbol{\alpha})$ be a "uniform" constant of motion, meaning that it is single valued and analytic in the non-simply-connected region $U \times \mathbb{T}^\ell$ and, for ε small,

$$B(\varepsilon, \boldsymbol{A}, \boldsymbol{\alpha}) = B_0(\boldsymbol{A}, \boldsymbol{\alpha}) + \varepsilon B_1(\boldsymbol{A}, \boldsymbol{\alpha}) + \varepsilon^2 B_2(\boldsymbol{A}, \boldsymbol{\alpha}) + \cdots \qquad [63]$$

The condition that B is a constant of motion can be written order by order in its expansion in ε: the first two orders are

$$\begin{aligned} &\boldsymbol{\omega}(\boldsymbol{A}) \cdot \partial_{\boldsymbol{\alpha}} B_0(\boldsymbol{A}, \boldsymbol{\alpha}) = 0 \\ &\partial_{\boldsymbol{A}} f(\boldsymbol{A}, \boldsymbol{\alpha}) \cdot \partial_{\boldsymbol{\alpha}} B_0(\boldsymbol{A}, \boldsymbol{\alpha}) - \partial_{\boldsymbol{\alpha}} f(\boldsymbol{A}, \boldsymbol{\alpha}) \cdot \partial_{\boldsymbol{A}} B_0(\boldsymbol{A}, \boldsymbol{\alpha}) \\ &\quad + \boldsymbol{\omega}(\boldsymbol{A}) \cdot \partial_{\boldsymbol{\alpha}} B_1(\boldsymbol{A}, \boldsymbol{\alpha}) = 0 \end{aligned} \qquad [64]$$

Then the above two relations and anisochrony imply (1) that B_0 must be a function of A only and (2) that $\omega(A)\cdot\nu$ and $\partial_A B_0(A)\cdot\nu$ vanish simultaneously for all ν. Hence, the gradient of B_0 must be proportional to $\omega(A)$, that is, to the gradient of $h(A)$: $\partial_A B_0(A) = \lambda(A)\partial_A h(A)$. Therefore, generically (because of the anisochrony) it must be that B_0 depends on A through $h(A)$: $B_0(A) = F(h(A))$ for some F.

Looking again, with the new information, at the second of [64] it follows that at fixed A the α-derivative in the direction $\omega(A)$ of B_1 equals $F'(h(A))$ times the α-derivative of f, that is, $B_1(A,\alpha) = f(A,\alpha)F'(h(A)) + C_1(A)$.

Summarizing: the constant of motion B has been written as $B(A,\alpha) = F(h(A)) + \varepsilon F'(h(A))f(A,\alpha) + \varepsilon C_1(A) + \varepsilon^2 B_2 + \cdots$ which is equivalent to $B(A,\alpha) = F(\mathcal{H}_\varepsilon) + \varepsilon(B_0' + \varepsilon B_1' + \cdots)$ and therefore $B_0' + \varepsilon B_1' + \cdots$ is another analytic constant of motion. Repeating the argument also $B_0' + \varepsilon B_1' + \cdots$ must have the form $F_1(\mathcal{H}_\varepsilon) + \varepsilon(B_0'' + \varepsilon B_1'' + \cdots)$; conclusion

$$B = F(\mathcal{H}_\varepsilon) + \varepsilon F_1(\mathcal{H}_\varepsilon) + \varepsilon^2 F_2(\mathcal{H}_\varepsilon) + \cdots + \varepsilon^n F_n(\mathcal{H}_\varepsilon) + O(\varepsilon^{n+1}) \qquad [65]$$

By analyticity, $B = F_\varepsilon(\mathcal{H}_\varepsilon(A,\alpha))$ for some F_ε: hence generically all constants of motion are trivial.

Therefore, a system close to integrable cannot behave as it would naively be expected. The problem, however, was not manifest until POINCARÉ's proof of the above results: because in most applications the function f has only finitely many Fourier components, or at least is replaced by an approximation with this property, so that at least [62] and even a few of the higher-order constraints like [64] become possible in open regions of action space. In fact, it may happen that the values of A of interest are restricted so that $\omega(A)\cdot\nu = 0$ only for "large" values of ν for which $f_\nu = 0$. Nevertheless, the property that $f_\nu(A) = (\omega(A)\cdot\nu)\tilde{f}_\nu(A)$ (or the analogous higher-order conditions, e.g., [64]), which we have seen to be necessary for analytic integrability of the perturbed system, can be checked to fail in important problems, if no approximation is made on f. Hence a conceptual problem arises.

For more details see Poincaré (1987).

Perturbing Functions

To check, in a given problem, the nonexistence of nontrivial constants of motion along the lines indicated in the previous section, it is necessary to express the potential, usually given in Cartesian coordinates as $\varepsilon V(x)$, in terms of the action–angle variables of the unperturbed, integrable, system.

In particular, the problem arises when trying to check nonexistence of nontrivial constants of motion when the anisochrony assumption (cf. the previous section) is not satisfied. Usually it becomes satisfied "to second order" (or higher): but to show this, a more detailed information on the structure of the perturbing function expressed in action–angle variables is needed. For instance, this is often necessary even when the perturbation is approximated by a trigonometric polynomial, as it is essentially always the case in celestial mechanics.

Finding explicit expressions for the action–angle variables is in itself a rather nontrivial task which leads to many problems of intrinsic interest even in seemingly simple cases. For instance, in the case of the planar gravitational central motion, the Kepler equation $\lambda = \xi - \varepsilon\sin\xi$ (see the first of [41]) must be solved expressing ξ in terms of λ (see the first of [42]). It is obvious that for small ε, the variable ξ can be expressed as an analytic function of ε: nevertheless, the actual construction of this expression leads to several problems. For small ε, an interesting algorithm is the following.

Let $h(\lambda) = \xi - \lambda$, so that the equation to solve (i.e., the first of [41]) is

$$h(\lambda) = \varepsilon\sin(\lambda + h(\lambda)) \equiv -\varepsilon\frac{\partial c}{\partial\lambda}(\lambda + h(\lambda)) \qquad [66]$$

where $c(\lambda) = \cos\lambda$; the function $\lambda \to h(\lambda)$ should be periodic in λ, with period 2π, and analytic in ε, λ for ε small and λ real. If $h(\lambda) = \varepsilon h^{(1)} + \varepsilon^2 h^{(2)} + \cdots$, the Fourier transform of $h^{(k)}(\lambda)$ satisfies the recursion relation

$$h_\nu^{(k)} = -\sum_{p=1}^{\infty}\frac{1}{p!}\sum_{\substack{k_1+\cdots+k_p=k-1\\ \nu_0+\nu_1+\cdots+\nu_p=\nu}} (\mathrm{i}\nu_0)c_{\nu_0}(\mathrm{i}\nu_0)^p \times\prod h_{\nu_j}^{(k_j)}, \quad k>1 \qquad [67]$$

with c_ν the Fourier transform of the cosine ($c_{\pm1} = \frac{1}{2}$, $c_\nu = 0$ if $\nu \neq \pm 1$), and (of course) $h_\nu^{(1)} = -\mathrm{i}\nu c_\nu$. Equation [67] is obtained by expanding the RHS of [66] in powers of h and then taking the Fourier transform of both sides retaining only terms of order k in ε.

Iterating the above relation, imagine drawing all trees θ with k "branches," or "lines," distinguished by a label taking k values, and k nodes and attach to each node v a harmonic label $\nu_v = \pm 1$ as in **Figure 5**. The trees will be assumed to start with a root line vr linking a point r and the "first node" v (see **Figure 5**)

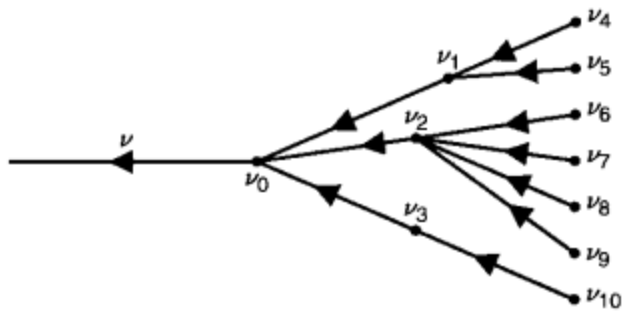

Figure 5 An example of a tree graph and its labels. It contains only one simple node (3). Harmonics are indicated next to their nodes. Labels distinguishing lines are not marked.

and then bifurcate arbitrarily (such trees are sometimes called "rooted trees").

Imagine the tree oriented from the endpoints towards the root r (not to be considered a node) and given a node v call v' the node immediately following it. If v is the first node before the root r, let $v'=r$ and $\nu_{v'}=1$. For each such decorated tree define its numerical value

$$\mathrm{Val}(\theta)=\frac{-\mathrm{i}}{k!}\prod_{\text{lines } l=v'v}(\nu_{v'}\nu_v)\prod_{\text{nodes}}c_{\nu_v} \qquad [68]$$

and define a current $\nu(l)$ on a line $l=v'v$ to be the sum of the harmonics of the nodes preceding v': $\nu(l)=\sum_{w\le v}\nu_v$. Call $\nu(\theta)$ the current flowing in the root branch and call order of θ the number of nodes (or branches). Then

$$h_\nu^{(k)}=\sum_{\substack{\theta,\nu(\theta)=\nu\\ \mathrm{order}(\theta)=k}}\mathrm{Val}(\theta) \qquad [69]$$

provided trees are considered identical if they can be overlapped (labels included) after suitably scaling the lengths of their branches and pivoting them around the nodes out of which they emerge (the root is always imagined to be fixed at the origin).

If the trees are stripped of the harmonic labels, their number is finite and it can be estimated to be $\le k!4^k$ (because the labels which distinguish the lines can be attached to an unlabeled tree in many ways). The harmonic labels (i.e., $\nu_v=\pm1$) can be laid down in 2^k ways, and the value of each tree can be bounded by $(1/k!)2^{-k}$ (because $c_{\pm1}=\frac{1}{2}$).

Hence $\sum_\nu|h_\nu^{(k)}|\le 4^k$, which gives a (rough) estimate of the radius of convergence of the expansion of h in powers of ε: namely 0.25 (easily improvable to 0.3678 if $4^kk!$ is replaced by k^{k-1} using Cayley's formula for the enumeration of rooted trees). A simple expression for $h^{(k)}(\psi)$ (LAGRANGE) is

$$h^{(k)}(\psi)=\frac{1}{k!}\partial_\psi^{k-1}\sin^k\psi$$

(also readable from the tree representation): the actual radius of convergence, first determined by Laplace, of the series for h can also be determined from the latter expression for h (ROUCHÉ) or directly from the tree representation: it is ~0.6627.

One can find better estimates or at least more efficient methods for evaluating the sums in [69]: in fact, in performing the sum in [69] important cancellations occur. For instance, the harmonic labels can be subject to the further strong constraint that no line carries zero current because the sum of the values of the trees of fixed order and with at least one line carrying zero current vanishes.

The above expansion can also be simplified by *partial resummations*. For the purpose of an example, let the nodes with one entering and one exiting line (see **Figure 5**) be called as "simple" nodes. Then all tree graphs which, on any line between two nonsimple nodes, contain any number of simple nodes can be eliminated. This is done by replacing, in evaluating the (remaining) tree values, the factors $\nu_{v'}\nu_v$ in [68] by $\nu_{v'}\nu_v/(1-\varepsilon\cos\psi)$: then the value of θ (denoted $\mathrm{Val}(\theta)_\psi$) for a tree becomes a function of ψ and ε and [69] is replaced by

$$h(\psi)=\sum_{k=1}^{\infty}\sum_{\substack{\theta,\nu(\theta)=\nu\\ \mathrm{order}(\theta)=k}}^{*}\varepsilon^k\,\mathrm{e}^{\mathrm{i}\nu\psi}\mathrm{Val}(\theta)_\psi \qquad [70]$$

where the $*$ means that the trees are subject to the further restriction of not containing any simple node. It should be noted that the above graphical representation of the solution of the Kepler equation is strongly reminiscent of the representations of quantities in terms of graphs that occur often in quantum field theory. Here the trees correspond to *Feynman graphs*, the factors associated with the nodes are the *couplings*, the factors associated with the lines are the *propagators*, and the resummations are analogous to the *self-energy resummations*, while the cancellations mentioned above can be related to the class of identities called *Ward identities*. Not only the analogy can be shown not to be superficial, but it also turns out to be very helpful in key mechanical problems: see Appendix 1.

The existence of a vast number of identities relating the tree values is shown already by the *simple* form of the Lagrange series and by the even more remarkable resummation (LEVI-CIVITA) leading to

$$h(\psi)=\sum_{k=1}^{\infty}\frac{(\varepsilon\sin\psi)^k}{k!}\left(\frac{1}{1-\varepsilon\cos\psi}\partial_\psi\right)^k\psi \qquad [71]$$

It is even possible to further collect the series terms to express it as a series with much better convergence properties; for instance, its terms can be reorganized and collected (resummed) so that h is expressed as a power series in the parameter

$$\eta = \frac{\varepsilon\, e^{\sqrt{1-\varepsilon^2}}}{1+\sqrt{1-\varepsilon^2}} \qquad [72]$$

with radius of convergence 1, which corresponds to $\varepsilon = 1$ (via a simple argument by Levi-Civita). The analyticity domain for the Lagrange series is $|\eta| < 1$. This also determines the value of Laplace radius, which is the point closest to the origin of the complex curve $|\eta(\varepsilon)| = 1$: it is imaginary so that it is the root of the equation

$$\varepsilon e^{\sqrt{1+\varepsilon^2}}/(1+\sqrt{1+\varepsilon^2}) = 1$$

The analysis provides an example, in a simple case of great interest in applications, of the kind of computations actually necessary to represent the perturbing function in terms of action–angle variables. The property that the function $c(\lambda)$ in [66] is the cosine has been used only to limit the range of the label ν to be ± 1; hence the same method, with similar results, can be applied to study the inversion of the relation between the average anomaly λ and the true anomaly θ and to efficiently obtain, for instance, the properties of f, g in [42].

For more details, the reader is referred to Levi-Civita (1956).

Lindstedt and Birkhoff Series: Divergences

Nonexistence of constants of motion, rather than being the end of the attempts to study motions close to integrable ones by perturbation methods, marks the beginning of renewed efforts to understand their nature.

Let $(\boldsymbol{A}, \boldsymbol{\alpha}) \in U \times \mathbb{T}^\ell$ be action–angle variables defined in the integrability region for an analytic Hamiltonian and let $h(\boldsymbol{A})$ be its value in the action–angle coordinates. Suppose that $h(\boldsymbol{A}_0)$ is anisochronous and let $f(\boldsymbol{A}, \boldsymbol{\alpha})$ be an analytic perturbing function. Consider, for ε small, the Hamiltonian $\mathcal{H}_\varepsilon(\boldsymbol{A}, \boldsymbol{\alpha}) = \mathcal{H}_0(\boldsymbol{A}) + \varepsilon f(\boldsymbol{A}, \boldsymbol{\alpha})$.

Let $\boldsymbol{\omega}_0 = \boldsymbol{\omega}(\boldsymbol{A}_0) \equiv \partial_{\boldsymbol{A}} \mathcal{H}_0(\boldsymbol{A})$ be the frequency spectrum (see the section "Quasiperiodicity and integrability") of one of the invariant tori of the unperturbed system corresponding to an action $\boldsymbol{A}_0$. Short of integrability, the question to ask at this point is whether the perturbed system admits an analytic invariant torus on which the motion is quasiperiodic and

1. has the same spectrum $\boldsymbol{\omega}_0$,
2. depends analytically on ε at least for ε small,
3. reduces to the "unperturbed torus" $\{\boldsymbol{A}_0\} \times \mathbb{T}^\ell$ as $\varepsilon \to 0$.

More concretely, the question is:

Are there functions $\boldsymbol{H}_\varepsilon(\boldsymbol{\psi}), \boldsymbol{h}_\varepsilon(\boldsymbol{\psi})$ analytic in $\boldsymbol{\psi} \in \mathbb{T}^\ell$ and in ε near 0, vanishing as $\varepsilon \to 0$ and such that the torus with parametric equations

$$\boldsymbol{A} = \boldsymbol{A}_0 + \boldsymbol{H}_\varepsilon(\boldsymbol{\psi}),\ \boldsymbol{\alpha} = \boldsymbol{\psi} + \boldsymbol{h}_\varepsilon(\boldsymbol{\psi}), \quad \boldsymbol{\psi} \in \mathbb{T}^\ell \qquad [73]$$

is invariant and, if $\boldsymbol{\omega}_0 \stackrel{\text{def}}{=} \boldsymbol{\omega}(\boldsymbol{A}_0)$, the motion on it is simply $\boldsymbol{\psi} \to \boldsymbol{\psi} + \boldsymbol{\omega}_0 t$, i.e., it is quasiperiodic with spectrum $\boldsymbol{\omega}_0$?

In this context, Poincaré's theorem (in the section "Generic nonintegrability") had followed another key result, earlier developed in particular cases and completed by him, which provides a partial answer to the question.

Suppose that $\boldsymbol{\omega}_0 = \boldsymbol{\omega}(\boldsymbol{A}_0) \in \mathbb{R}^\ell$ satisfies a Diophantine property, namely suppose that there exist constants $C, \tau > 0$ such that

$$|\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}| \geq \frac{1}{C|\boldsymbol{\nu}|^\tau}, \quad \text{for all } 0 \neq \boldsymbol{\nu} \in \mathbb{Z}^\ell \qquad [74]$$

which, for each $\tau > \ell - 1$ fixed, is a property enjoyed by all $\boldsymbol{\omega} \in \mathbb{R}^\ell$ but for a set of zero measure. Then the motions on the unperturbed torus run over trajectories that fill the torus densely because of the "irrationality" of $\boldsymbol{\omega}_0$ implied by [74]. Writing Hamilton's equations,

$$\dot{\boldsymbol{\alpha}} = \partial_{\boldsymbol{A}} \mathcal{H}_0(\boldsymbol{A}) + \varepsilon \partial_{\boldsymbol{A}} f(\boldsymbol{A}, \boldsymbol{\alpha}), \quad \dot{\boldsymbol{A}} = -\varepsilon \partial_{\boldsymbol{\alpha}} f(\boldsymbol{A}, \boldsymbol{\alpha})$$

with $\boldsymbol{A}, \boldsymbol{\alpha}$ given by [73] with $\boldsymbol{\psi}$ replaced by $\boldsymbol{\psi} + \boldsymbol{\omega} t$, and using the density of the unperturbed trajectories implied by [74], the condition that [73] are equations for an invariant torus on which the motion is $\boldsymbol{\psi} \to \boldsymbol{\psi} + \boldsymbol{\omega}_0 t$ are

$$\begin{aligned} \boldsymbol{\omega}_0 + (\boldsymbol{\omega}_0 \cdot \partial_{\boldsymbol{\psi}}) \boldsymbol{h}_\varepsilon(\boldsymbol{\psi}) &= \partial_{\boldsymbol{A}} \mathcal{H}_0(\boldsymbol{A}_0 + \boldsymbol{H}_\varepsilon(\boldsymbol{\psi})) \\ &+ \varepsilon \partial_{\boldsymbol{A}} f(\boldsymbol{A}_0 + \boldsymbol{H}_\varepsilon(\boldsymbol{\psi}), \boldsymbol{\psi} + \boldsymbol{h}_\varepsilon(\boldsymbol{\psi}))(\boldsymbol{\omega}_0 \cdot \partial_{\boldsymbol{\psi}}) \boldsymbol{H}_\varepsilon(\boldsymbol{\psi}) \\ &= -\varepsilon \partial_{\boldsymbol{\alpha}} f(\boldsymbol{A}_0 + \boldsymbol{H}_\varepsilon(\boldsymbol{\psi}), \boldsymbol{\psi} + \boldsymbol{h}_\varepsilon(\boldsymbol{\psi})) \end{aligned} \qquad [75]$$

The theorem referred to above (POINCARÉ) is that

Theorem 2 *If the unperturbed system is anisochronous and $\boldsymbol{\omega}_0 = \boldsymbol{\omega}(\boldsymbol{A}_0)$ satisfies* [74] *for some $C, \tau > 0$ there exist two well defined power series $\boldsymbol{h}_\varepsilon(\boldsymbol{\psi}) = \sum_{k=1}^\infty \varepsilon^k \boldsymbol{h}^{(k)}(\boldsymbol{\psi})$ and $\boldsymbol{H}_\varepsilon(\boldsymbol{\psi}) = \sum_{k=1}^\infty \varepsilon^k \boldsymbol{H}^{(k)}(\boldsymbol{\psi})$ which*

solve [75] *to all orders in* ε. *The series for* $\boldsymbol{H}_\varepsilon$ *is uniquely determined, and such is also the series for* $\boldsymbol{h}_\varepsilon$ *up to the addition of an arbitrary constant at each order, so that it is unique if* $\boldsymbol{h}_\varepsilon$ *is required, as henceforth done with no loss of generality, to have zero average over* $\boldsymbol{\psi}$.

The algorithm for the construction is illustrated in a simple case in the next section (see eqns [83], [84]). Convergence of the above series, called *Lindstedt series*, even for small ε has been a problem for rather a long time. Poincaré proved the existence of the formal solution; but his other result, discussed in the section "Generic nonintegrability," casts doubts on convergence although it does not exclude it, as was immediately stressed by several authors (including Poincaré himself). The result in that section shows the impossibility of solving [75] for all $\boldsymbol{\omega}_0$'s near a given spectrum, analytically and uniformly, but it does not exclude the possibility of solving it for a single $\boldsymbol{\omega}_0$.

The theorem admits several extensions or analogs: an interesting one is to the case of isochronous unperturbed systems:

> Given the Hamiltonian $\mathcal{H}_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha}) = \boldsymbol{\omega}_0 \cdot \boldsymbol{A} + \varepsilon f(\boldsymbol{A},\boldsymbol{\alpha})$, with $\boldsymbol{\omega}_0$ satisfying [74] and f analytic, there exist power series $\mathcal{C}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}')$, $u_\varepsilon(\boldsymbol{A}')$ such that $\mathcal{H}_\varepsilon(\mathcal{C}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}')) = \boldsymbol{\omega}_0 \cdot \boldsymbol{A}' + u_\varepsilon(\boldsymbol{A}')$ holds as an equality between formal power series (i.e., order by order in ε) and at the same time the $\mathcal{C}_\varepsilon$, regarded as a map, satisfies order by order the condition (i.e., (4.3)) that it is a canonical map.

This means that there is a generating function $\boldsymbol{A}' \cdot \boldsymbol{\alpha} + \boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha})$ also defined by a formal power series $\boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}) = \sum_{k=1}^{\infty} \varepsilon^k \boldsymbol{\Phi}^{(k)}(\boldsymbol{A}',\boldsymbol{\alpha})$, that is, such that if $\mathcal{C}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}') = (\boldsymbol{A},\boldsymbol{\alpha})$ then it is true, order by order in powers of ε, that $\boldsymbol{A} = \boldsymbol{A}' + \partial_{\boldsymbol{\alpha}} \boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha})$ and $\boldsymbol{\alpha}' = \boldsymbol{\alpha} + \partial_{\boldsymbol{A}'} \boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha})$. The series for $\boldsymbol{\Phi}_\varepsilon, u_\varepsilon$ are called Birkhoff series.

In this isochronous case, if Birkhoff series were convergent for small ε and $(\boldsymbol{A}',\boldsymbol{\alpha})$ in a region of the form $U \times \mathbb{T}^\ell$, with $U \subset \mathbb{R}^\ell$ open and bounded, it would follow that, for small ε, $\mathcal{H}_\varepsilon$ would be integrable in a large region of phase space (i.e., where the generating function can be used to build a canonical map: this would essentially be $U \times \mathbb{T}^\ell$ deprived of a small layer of points near the boundary of U). However, convergence for small ε is false (in general), as shown by the simple two-dimensional example

$$\begin{aligned} &\mathcal{H}_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha}) = \boldsymbol{\omega}_0 \cdot \boldsymbol{A} + \varepsilon\,(A_2 + f(\boldsymbol{\alpha})) \\ &(\boldsymbol{A},\boldsymbol{\alpha}) \in \mathbb{R}^2 \times \mathbb{T}^2 \end{aligned} \qquad [76]$$

with $f(\boldsymbol{\alpha})$ an arbitrary analytic function with all Fourier coefficients f_ν positive for $\boldsymbol{\nu} \neq 0$ and $f_0 = 0$. In the latter case, the solution is

$$\begin{aligned} &u_\varepsilon(\boldsymbol{A}') = \varepsilon A_2 \\ &\boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}) = \\ &\qquad \sum_{k=1}^{\infty} \varepsilon^k \sum_{0 \neq \boldsymbol{\nu} \in \mathbb{Z}^2} f_{\boldsymbol{\nu}}\, \mathrm{e}^{\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{\nu}} \frac{(\mathrm{i}\,\nu_2)^k}{(\mathrm{i}(\omega_{01}\nu_1 + \omega_{02}\nu_2))^{k+1}} \end{aligned} \qquad [77]$$

The series does not converge: in fact, its convergence would imply integrability and, consequently, bounded trajectories in phase space: however, the equations of motion for [76] can be easily solved explicitly and in any open region near given initial data there are other data which have unbounded trajectories if $\omega_{01}/(\omega_{02} + \varepsilon)$ is rational.

Nevertheless, even in this elementary case a formal sum of the series yields

$$\begin{aligned} &u(\boldsymbol{A}') = \varepsilon A_2' \\ &\boldsymbol{\Phi}_\varepsilon(\boldsymbol{A}',\boldsymbol{\alpha}) = \varepsilon \sum_{0 \neq \boldsymbol{\nu} \in \mathbb{Z}^2} \frac{f_{\boldsymbol{\nu}}\, \mathrm{e}^{\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{\nu}}}{\mathrm{i}(\omega_{01}\nu_1 + (\omega_{20} + \varepsilon)\nu_2)} \end{aligned} \qquad [78]$$

and the series in [78] (no longer a power series in ε) is really convergent if $\boldsymbol{\omega} = (\omega_{01}, \omega_{02} + \varepsilon)$ is a Diophantine vector (by [74], because analyticity implies exponential decay of $|f_\nu|$). Remarkably, for such values of ε the Hamiltonian $\mathcal{H}_\varepsilon$ is integrable and it is integrated by the canonical map generated by [78], in spite of the fact that [78] is obtained, from [77], via the nonrigorous sum rule

$$\sum_{k=0}^{\infty} z^k = \frac{1}{1-z} \quad \text{for } z \neq 1 \qquad [79]$$

(applied to cases with $|z| \geq 1$, which are certainly realized for a dense set of ε's even if $\boldsymbol{\omega}$ is Diophantine because the z's have values $z = \nu_2/\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}$). In other words, the integration of the equations is elementary and once performed it becomes apparent that, if $\boldsymbol{\omega}$ is diophantine, the solutions can be rigorously found from [78]. Note that, for instance, this means that relations like $\sum_{k=0}^{\infty} 2^k = -1$ are really used to obtain [78] from [77].

Another extension of Lindstedt series arises in a perturbation of an anisochronous system when asking the question as to what happens to the unperturbed invariant tori $\mathcal{T}_{\boldsymbol{\omega}_0}$ on which the spectrum is resonant, that is, $\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu} = 0$ for some $\boldsymbol{\nu} \neq 0$, $\boldsymbol{\nu} \in \mathbb{Z}^\ell$. The result is that even in such a case there is a formal power series solution showing that at least a few of the (infinitely many) invariant tori into which $\mathcal{T}_{\boldsymbol{\omega}_0}$ is in turn foliated in the unperturbed case can be formally continued at $\varepsilon \neq 0$ (see the section "Resonances and their stability").

For more details, we refer the reader to Poincaré (1987).

Quasiperiodicity and KAM Stability

To discuss more advanced results, it is convenient to restrict attention to a special (nontrivial) paradigmatic case

$$\mathcal{H}_\varepsilon(A,\alpha) = \tfrac{1}{2}A^2 + \varepsilon f(\alpha) \qquad [80]$$

In this simple case (called *Thirring model*: representing ℓ particles on a circle interacting via a potential $\varepsilon f(\alpha)$) the equations for the maximal tori [75] reduce to equations for the only functions h_ε:

$$(\omega\cdot\partial_\psi)^2 h_\varepsilon(\psi) = -\varepsilon\partial_\alpha f(\psi + h_\varepsilon(\psi)), \quad \psi\in\mathbb{T}^\ell \qquad [81]$$

as the second of [75] simply becomes the definition of H_ε because the RHS does not involve H_ε.

The real problem is therefore whether the formal series considered in the last section converge at least for small ε: and the example [76] on the Birkhoff series shows that sometimes sum rules might be needed in order to give a meaning to the series. In fact, whenever a problem (of physical interest) admits a formal power series solution which is not convergent, or which is such that it is not known whether it is convergent, then one should look for sum rules for it.

The modern theory of perturbations starts with the proof of the convergence for ε small enough of the Lindstedt series (KOLMOGOROV). The general "KAM" result is:

Theorem 3 (KAM) *Consider the Hamiltonian* $\mathcal{H}_\varepsilon(A,\alpha) = h(A) + \varepsilon f(A,\alpha)$, *defined in* $U = V\times\mathbb{T}^\ell$ *with* $V\subset\mathbb{R}^\ell$ *open and bounded and with* $f(A,\alpha)$, $h(A)$ *analytic in the closure* $\overline{V}\times\mathbb{T}^\ell$ *where* $h(A)$ *is also anisochronous; let* $\omega_0 \stackrel{\text{def}}{=} \omega(A_0) = \partial_A h(A_0)$ *and assume that* ω_0 *satisfies* [74]. *Then*

(i) *there is* $\varepsilon_{C,\tau} > 0$ *such that the Lindstedt series converges for* $|\varepsilon| < \varepsilon_{C,\tau}$;
(ii) *its sum yields two function* $H_\varepsilon(\psi), h_\varepsilon(\psi)$ *on* $\mathbb{T}^\ell$ *which parametrize an invariant torus* $\mathcal{T}_{C,\tau}(A_0,\varepsilon)$;
(iii) *on* $\mathcal{T}_{C,\tau}(A_0,\varepsilon)$ *the motion is* $\psi\to\psi+\omega_0 t$, *see* [73]; *and*
(iv) *the set of data in U which belong to invariant tori* $\mathcal{T}_{C,\tau}(A_0,\varepsilon)$ *with* $\omega(A_0)$ *satisfying* [74] *with prefixed* C,τ *has complement with volume* $<\text{const}\, C^{-a}$ *for a suitable* $a>0$ *and with area also* $<\text{const}\ C^{-a}$ *on each nontrivial surface of constant energy* $\mathcal{H}_\varepsilon = E$.

In other words, for small ε the spectra of most unperturbed quasiperiodic motions can still be found as spectra of perturbed quasiperiodic motions developing on tori which are close to the corresponding unperturbed ones (i.e., with the same spectrum).

This is a stability result: for instance, in systems with two degrees of freedom the invariant tori of dimension two which lie on a given three-dimensional energy surface, will separate the points on the energy surface into the set which is "inside" the torus and the set which is "outside." Hence, an initial datum starting (say) inside cannot reach the outside. Likewise, a point starting between two tori has to stay in between forever. Further, if the two tori are close, this means that motion will stay very localized in action space, with a trajectory accessing only points close to the tori and coming close to all such points, within a distance of the order of the distance between the confining tori. The case of three or more degrees of freedom is quite different (see sections "Diffusion in phase space" and "The three-body problem").

In the simple case of the rotators system [80] the equations for the parametric representation of the tori are given by [81]. The latter bear some analogy with the easier problem in [66]: but [81] are ℓ equations instead of one and they are differential equations rather than ordinary equations. Furthermore, the function $f(\alpha)$ which plays here the role of $c(\lambda)$ in [66] has Fourier coefficient f_ν with no restrictions on ν, while the Fourier coefficients c_ν for c in [66] do not vanish only for $\nu = \pm 1$.

The above differences are, to some extent, "minor" and the power series solution to [81] can be constructed by the same algorithm as used in the case of [66]: namely one forms trees as in **Figure 5** with the harmonic labels $\nu_v\in\mathbb{Z}$ replaced by $\nu_v\in\mathbb{Z}^\ell$ (still to be thought of as possible harmonic indices in the Fourier expansion of the perturbing function f). All other labels affixed to the trees in the section "Generic nonintegrability" will be the same. In particular, the current flowing on a branch $l = v'v$ will be defined as the sum of the harmonics of the nodes $w\le v$ preceding v:

$$\nu(l) \stackrel{\text{def}}{=} \sum_{w\le v} \nu_w \qquad [82]$$

and we call $\nu(\theta)$ the current flowing in the root branch.

Here the value $\text{Val}(\theta)$ of a tree has to be defined differently because the equation to be solved ([81]) contains the differential operator $(\omega_0\cdot\partial_\psi)^2$ which, when Fourier transformed, becomes multiplication of the Fourier component with harmonic ν by $(i\omega\cdot\nu)^2$.

The variation due to the presence of the operator $(\omega_0\cdot\partial_\psi)^2$ and the necessity of its inversion in the evaluation of $u\cdot h_\nu^{(k)}$, that is, of the component of $h_\nu^{(k)}$ along an arbitrary unit vector u, is nevertheless quite simple: the value of a tree graph θ of order k

(i.e., with k nodes and k branches) has to be defined by (cf. [68])

$$\mathrm{Val}(\theta) \stackrel{\text{def}}{=} \frac{-\mathrm{i}(-1)^k}{k!}\left(\prod_{\text{lines } l=v'v}\frac{\nu_{v'}\cdot\nu_v}{(\omega_0\cdot\nu(l))^2}\right) \times\left(\prod_{\text{nodes } v} f_{\nu_v}\right) \qquad [83]$$

where the $\nu_{v'}$ appearing in the factor relative to the root line rv from the first node v to the root r (see **Figure 5**) is interpreted as a unit vector $\boldsymbol{u}$ (it was interpreted as 1 in the one-dimensional case [66]). Equation [83] makes sense only for trees in which no line carries zero current. Then the component along $\boldsymbol{u}$ (the harmonic label attached to the root of a tree) of $\boldsymbol{h}^{(k)}$ is given (see also [69]) by

$$\boldsymbol{u}\cdot\boldsymbol{h}_\nu^{(k)} = \sum_{\substack{\theta,\,\nu(\theta)=\nu\\ \mathrm{order}(\theta)=k}}^{*}\mathrm{Val}(\theta) \qquad [84]$$

where the $*$ means that the sum is only over trees in which a nonzero current $\nu(l)$ flows on the lines $l\in\theta$. The quantity $\boldsymbol{u}\cdot\boldsymbol{h}_0^{(k)}$ will be defined to be 0 (see the previous section).

In the case of [66] zero-current lines could appear: but the contributions from tree graphs containing at least one zero current line would cancel. In the present case, the statement that the above algorithm actually gives $\boldsymbol{h}_\nu^{(k)}$ by simply ignoring trees with lines with zero current is nontrivial. It was Poincaré's contribution to the theory of Lindstedt series to show that even in the general case (cf. [75]) the equations for the invariant tori can be solved by a formal power series. Equation [84] is proved by induction on k after checking it for the first few orders.

The algorithm just described leading to [83] can be extended to the case of the general Hamiltonian considered in the KAM theorem.

The convergence proof is more delicate than the (elementary) one for eqn [66]. In fact, the values of trees of order k can give large contributions to $\boldsymbol{h}_\nu^{(k)}$: because the "new" factors $(\omega_0\cdot\nu(l))^2$, although not zero, can be quite small and their small size can overwhelm the smallness of the factors f_ν and ε. In fact, even if f is a trigonometric polynomial (so that f_ν vanishes identically for $|\nu|$ large enough) the currents flowing in the branches can be very large, of the order of the number k of nodes in the tree; see [82].

This is called the *small-divisors problem*. The key to its solution goes back to a related work (SIEGEL) which shows that

Theorem 4 *Consider the contribution to the sum in* [82] *from graphs θ in which no pairs of lines which lie on the same path to the root carry the same current and, furthermore, the node harmonics are bounded by $|\nu|\le N$ for some N. Then the number of lines ℓ in θ with divisor $\omega_0\cdot\nu_\ell$ satisfying $2^{-n} < C|\omega_0\cdot\nu_\ell|\le 2^{-n+1}$ does not exceed $4Nk2^{-n/\tau}$.*

Hence, setting

$$F \stackrel{\text{def}}{=} C^2\max_{|\nu|\le N}|f_\nu|$$

the corresponding $\mathrm{Val}(\theta)$ can be bounded by

$$\frac{1}{k!}F^kN^{2k}\prod_{n=0}^{\infty}2^{2n(4Nk2^{n/\tau})} \stackrel{\text{def}}{=} \frac{1}{k!}B^k$$
$$B = FN^2 2\sum_n 8n2^{-n/\tau} \qquad [85]$$

since the product is convergent. In the case in which f is a trigonometric polynomial of degree N, the above restricted contributions to $\boldsymbol{u}\cdot\boldsymbol{h}_\nu^{(k)}$ would generate a convergent series for ε small enough. In fact, the number of trees is bounded (as in the section "Perturbing functions") by $k!4^k(2N+1)^{\ell k}$ so that the series $\sum_\nu|\varepsilon|^k|\boldsymbol{u}\cdot\boldsymbol{h}_\nu^{(k)}|$ would converge for small ε (i.e., $|\varepsilon| < (B\cdot 4(2N+1)^\ell)^{-1}$).

Given this comment, the analysis of the "remaining contributions" becomes the real problem, and it requires new ideas because among the excluded trees there are some simple kth order trees whose value alone, if considered separately from the other contributions, would generate a factorially divergent power series in ε.

However, the contributions of all large-valued trees of order k can be shown to cancel: although not exactly (unlike the case of the elementary problem in the section "Perturbing functions," where the cancellation is not necessary for the proof, in spite of its exact occurrence), but enough so that in spite of the existence of exceedingly large values of individual tree graphs their total sum can still be bounded by a constant to the power k so that the power series actually converges for ε small enough. The idea is discussed in Appendix 1.

For more details, the reader is referred to Poincaré (1987), Kolmogorov (1954), Moser (1962), and Arnol'd (1989).

Resonances and their Stability

A quasiperiodic motion with r rationally independent frequencies is called resonant if r is strictly less than the number of degrees of freedom, ℓ. The difference $s=\ell-r$ is the degree of the resonance.

Of particular interest are the cases of a perturbation of an integrable system in which resonant motions take place.

A typical example is the n-body problem which studies the mutual perturbations of the motions of $n-1$ particles gravitating around a more massive particle. If the particle masses can be considered to be negligible, the system will consist of $n-1$ central Keplerian motions: it will therefore have $\ell = 3(n-1)$ degrees of freedom. In general, only one frequency per body occurs in the absence of the perturbations (the period of the Keplerian orbit). Hence, $r \leq n-1$ and $s \geq 2(n-1)$ (or in the planar case $s \geq (n-1)$) with equality holding when the periods are rationally independent.

Another example is the rigid body with a fixed point perturbed by a conservative force: in this case, the unperturbed system has three degrees of freedom but, in general, only two frequencies (see the discussion following [52]).

Furthermore, in the above examples there is the possibility that the independent frequencies assume, for special initial data, values which are rationally related, giving rise to resonances of even higher order (i.e., with smaller values of r).

In an integrable anisochronous system, resonant motions will be dense in phase space because the frequencies $\boldsymbol{\omega}(\boldsymbol{A})$ will vary as much as the actions and therefore resonances of any order (i.e., any $r < \ell$) will be dense in phase space: in particular, the periodic motions (i.e., the highest-order resonances) will be dense.

Resonances, in integrable systems, can arise in *a priori* stable integrable systems and in *a priori* unstable systems: the former are systems whose Hamiltonian admits canonical action–angle coordinates $(\boldsymbol{A}, \boldsymbol{\alpha}) \in U \times \mathbb{T}^\ell$ with $U \subset \mathbb{R}^\ell$ open, while the latter are systems whose Hamiltonian has, in suitable local canonical coordinates, the form

$$\mathcal{H}_0(\boldsymbol{A}) + \sum_{i=1}^{s_1} \frac{1}{2}(p_i^2 - \lambda_i^2 q_i^2) + \sum_{j=1}^{s_2} \frac{1}{2}(\pi_j^2 + \mu_j^2 \kappa_j^2), \qquad \lambda_i, \mu_j > 0 \qquad [86]$$

where $(\boldsymbol{A}, \boldsymbol{\alpha}) \in U \times \mathbb{T}^r$, $U \in \mathbb{R}^r$, $(\boldsymbol{p}, \boldsymbol{q}) \in V \subset \mathbb{R}^{2s_1}$, $(\boldsymbol{\pi}, \boldsymbol{\kappa}) \in V' \subset \mathbb{R}^{2s_2}$ with V, V' neighborhoods of the origin and $\ell = r + s_1 + s_2$, $s_i \geq 0$, $s_1 + s_2 > 0$ and $\pm\sqrt{\lambda_j}$, $\pm\sqrt{\mu_j}$ are called Lyapunov coefficients of the resonance. The perturbations considered are supposed to have the form $\varepsilon f(\boldsymbol{A}, \boldsymbol{\alpha}, \boldsymbol{p}, \boldsymbol{q}, \boldsymbol{\pi}, \boldsymbol{\kappa})$. The denomination of *a priori* stable or unstable refers to the properties of the "*a priori* given unperturbed Hamiltonian." The label "*a priori* unstable" is certainly appropriate if $s_1 > 0$: here also $s_1 = 0$ is allowed for notational convenience implying that the Lyapunov coefficients in *a priori* unstable cases are all of order 1 (whether real λ_j or imaginary $i\sqrt{\mu_j}$). In other words, the *a priori* stable case, $s_1 = s_2 = 0$ in [86], is the only excluded case. Of course, the stability properties of the motions when a perturbation acts will depend on the perturbation in both cases.

The *a priori* stable systems usually have a great variety of resonances (e.g., in the anisochronous case, resonances of any dimension are dense). The *a priori* unstable systems have (among possible other resonances) some very special r-dimensional resonances occurring when the unstable coordinates $(\boldsymbol{p}, \boldsymbol{q})$ and $(\boldsymbol{\pi}, \boldsymbol{\kappa})$ are zero and the frequencies of the r action–angle coordinates are rationally independent.

In the first case (*a priori* stable), the general question is whether the resonant motions, which form invariant tori of dimension r arranged into families that fill ℓ-dimensional invariant tori, continue to exist, in presence of small enough perturbations $\varepsilon f(\boldsymbol{A}, \boldsymbol{\alpha})$, on slightly deformed invariant tori. Similar questions can be asked in the *a priori* unstable cases. To examine the matter more closely consider the formulation of the simplest problems.

A priori stable resonances: more precisely, suppose $\mathcal{H}_0 = \frac{1}{2}A^2$ and let $\{\boldsymbol{A}_0\} \times \mathbb{T}^\ell$ be the unperturbed invariant torus $\mathcal{T}_{\boldsymbol{A}_0}$ with spectrum $\boldsymbol{\omega}_0 = \boldsymbol{\omega}(\boldsymbol{A}_0) = \partial_{\boldsymbol{A}} \mathcal{H}_0(\boldsymbol{A}_0)$ with only r rationally independent components. For simplicity, suppose that $\boldsymbol{\omega}_0 = (\omega_1, \ldots, \omega_r, 0, \ldots, 0) \stackrel{\text{def}}{=} (\boldsymbol{\omega}, 0)$ with $\boldsymbol{\omega} \in \mathbb{R}^r$. The more general case in which $\boldsymbol{\omega}$ has only r rationally independent components can be reduced to the special case above by a canonical linear change of coordinates at the price of changing the $\mathcal{H}_0$ to a new one, still quadratic in the actions but containing mixed products $A_i B_j$: the proofs of the results that are discussed here would not be really affected by such more general form of $\mathcal{H}$.

It is convenient to distinguish between the "fast" angles $\alpha_1, \ldots, \alpha_r$ and the "resonant" angles $\alpha_{r+1}, \ldots, \alpha_\ell$ (also called "slow" or "secular") and call $\boldsymbol{\alpha} = (\boldsymbol{\alpha}', \boldsymbol{\beta})$ with $\boldsymbol{\alpha}' \in \mathbb{T}^r$ and $\boldsymbol{\beta} \in \mathbb{T}^s$. Likewise, we distinguish the fast actions $\boldsymbol{A}' = (A_1, \ldots, A_r)$ and the resonant ones $A_{r+1}, \ldots, A_\ell$ and set $\boldsymbol{A} = (\boldsymbol{A}', \boldsymbol{B})$ with $\boldsymbol{A}' \in \mathbb{R}^r$ and $\boldsymbol{B} \in \mathbb{R}^s$.

Therefore, the torus $\mathcal{T}_{\boldsymbol{A}_0}$, $\boldsymbol{A}_0 = (\boldsymbol{A}_0', \boldsymbol{B}_0)$, is in turn a continuum of invariant tori $\mathcal{T}_{\boldsymbol{A}_0, \boldsymbol{\beta}}$ with trivial parametric equations: $\boldsymbol{\beta}$ fixed, $\boldsymbol{\alpha}' = \boldsymbol{\psi}$, $\boldsymbol{\psi} \in \mathbb{T}^r$, and $\boldsymbol{A}' = \boldsymbol{A}_0'$, $\boldsymbol{B} = \boldsymbol{B}_0$. On each of them the motion is: $\boldsymbol{A}', \boldsymbol{B}, \boldsymbol{\beta}$ constant and $\boldsymbol{\alpha}' \to \boldsymbol{\alpha}' + \boldsymbol{\omega} t$, with rationally independent $\boldsymbol{\omega} \in \mathbb{R}^r$.

Then the natural question is whether there exist functions $\boldsymbol{h}_\varepsilon, \boldsymbol{k}_\varepsilon, \boldsymbol{H}_\varepsilon, \boldsymbol{K}_\varepsilon$ smooth in ε near $\varepsilon = 0$ and in $\boldsymbol{\psi} \in \mathbb{T}^r$, vanishing for $\varepsilon = 0$, and such that the torus $\mathcal{T}_{\boldsymbol{A}_0, \boldsymbol{\beta}_0, \varepsilon}$ with parametric equations

$$\begin{aligned} \boldsymbol{A}' &= \boldsymbol{A}_0' + \boldsymbol{H}_\varepsilon(\boldsymbol{\psi}), \quad & \boldsymbol{\alpha}' &= \boldsymbol{\psi} + \boldsymbol{h}_\varepsilon(\boldsymbol{\psi}), \\ \boldsymbol{B} &= \boldsymbol{B}_0 + \boldsymbol{K}_\varepsilon(\boldsymbol{\psi}), \quad & \boldsymbol{\beta} &= \boldsymbol{\beta}_0 + \boldsymbol{k}_\varepsilon(\boldsymbol{\psi}) \end{aligned} \qquad \boldsymbol{\psi} \in \mathbb{T}^r \qquad [87]$$

is invariant for the motions with Hamiltonian

$$\mathcal{H}_\varepsilon(\boldsymbol{A},\boldsymbol{\alpha}) = \tfrac{1}{2}\boldsymbol{A}'^2 + \tfrac{1}{2}\boldsymbol{B}^2 + \varepsilon f(\boldsymbol{\alpha}',\boldsymbol{\beta})$$

and the motions on it are $\boldsymbol{\psi} \to \boldsymbol{\psi} + \boldsymbol{\omega}t$. The above property, when satisfied, is summarized by saying that the unperturbed resonant motions $\boldsymbol{A} = (\boldsymbol{A}'_0, \boldsymbol{B}_0)$, $\boldsymbol{\alpha} = (\boldsymbol{\alpha}'_0 + \boldsymbol{\omega}'t, \boldsymbol{\beta}_0)$ can be continued in presence of perturbation εf, for small ε, to quasiperiodic motions with the same spectrum and on a slightly deformed torus $\mathcal{T}_{\boldsymbol{A}'_0,\boldsymbol{\beta}_0,\varepsilon}$.

A priori unstable resonances: here the question is whether the special invariant tori continue to exist in presence of small enough perturbations, of course slightly deformed. This means asking whether, given $\boldsymbol{A}_0$ such that $\boldsymbol{\omega}(\boldsymbol{A}_0) = \partial_{\boldsymbol{A}}\mathcal{H}_0(\boldsymbol{A}_0)$ has rationally independent components, there are functions $(\boldsymbol{H}_\varepsilon(\boldsymbol{\psi}), \boldsymbol{h}_\varepsilon(\boldsymbol{\psi}))$, $(\boldsymbol{P}_\varepsilon(\boldsymbol{\psi}), \boldsymbol{Q}_\varepsilon(\boldsymbol{\psi}))$ and $(\boldsymbol{\Pi}_\varepsilon(\boldsymbol{\psi}), \boldsymbol{K}_\varepsilon(\boldsymbol{\psi}))$ smooth in ε near $\varepsilon = 0$, vanishing for $\varepsilon = 0$, analytic in $\boldsymbol{\psi} \in \mathbb{T}^r$ and such that the r-dimensional surface

$$\begin{aligned} &\boldsymbol{A} = \boldsymbol{A}_0 + \boldsymbol{H}_\varepsilon(\boldsymbol{\psi}), \quad && \boldsymbol{\alpha} = \boldsymbol{\psi} + \boldsymbol{h}_\varepsilon(\boldsymbol{\psi}) \\ &\boldsymbol{p} = \boldsymbol{P}_\varepsilon(\boldsymbol{\psi}), && \boldsymbol{q} = \boldsymbol{Q}_\varepsilon(\boldsymbol{\psi}) \qquad \boldsymbol{\psi} \in \mathbb{T}^r \\ &\boldsymbol{\pi} = \boldsymbol{\Pi}_\varepsilon(\boldsymbol{\psi}), && \boldsymbol{\kappa} = \boldsymbol{K}_\varepsilon(\boldsymbol{\psi}) \end{aligned} \qquad [88]$$

is an invariant torus $\mathcal{T}_{\boldsymbol{A}_0,\varepsilon}$ on which the motion is $\boldsymbol{\psi} \to \boldsymbol{\psi} + \boldsymbol{\omega}(\boldsymbol{A}_0)t$. Again, the above property is summarized by saying that the unperturbed special resonant motions can be continued in presence of perturbation εf for small ε to quasiperiodic motions with the same spectrum and on a slightly deformed torus $\mathcal{T}_{\boldsymbol{A}_0,\varepsilon}$.

Some answers to the above questions are presented in the following section. For more details, the reader is referred to Gallavotti *et al.* (2004).

Resonances and Lindstedt Series

We discuss eqns [87] in the paradigmatic case in which the Hamiltonian $\mathcal{H}_0(\boldsymbol{A})$ is $\frac{1}{2}\boldsymbol{A}^2$ (cf. [80]). It will be $\boldsymbol{\omega}(\boldsymbol{A}') \equiv \boldsymbol{A}'$ so that $\boldsymbol{A}_0 = \boldsymbol{\omega}$, $\boldsymbol{B}_0 = 0$ and the perturbation $f(\boldsymbol{\alpha})$ can be considered as a function of $\boldsymbol{\alpha} = (\boldsymbol{\alpha}', \boldsymbol{\beta})$: let $\bar{f}(\boldsymbol{\beta})$ be defined as its average over $\boldsymbol{\alpha}'$. The determination of the invariant torus of dimension r which can be continued in the sense discussed in the last section is easily understood in this case.

A resonant invariant torus which, among the tori $\mathcal{T}_{\boldsymbol{A}_0,\boldsymbol{\beta}}$, has parametric equations that can be continued as a formal power series in ε is the torus $\mathcal{T}_{\boldsymbol{A}_0,\boldsymbol{\beta}_0}$ with $\boldsymbol{\beta}_0$ a stationarity point for $\bar{f}(\boldsymbol{\beta})$, that is, an equilibrium point for the average perturbation: $\partial_{\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0) = 0$. In fact, the following theorem holds:

Theorem 5 *If $\boldsymbol{\omega} \in \mathbb{R}^r$ satisfies a Diophantine property and if $\boldsymbol{\beta}_0$ is a nondegenerate stationarity point for the "fast angle average" $\bar{f}(\boldsymbol{\beta})$* (i.e., *such that* $\det \partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0) \neq 0$), *then the following equations for the functions $\boldsymbol{h}_\varepsilon, \boldsymbol{k}_\varepsilon$,*

$$\begin{aligned} (\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\psi}})^2\boldsymbol{h}_\varepsilon(\boldsymbol{\psi}) &= -\varepsilon\partial_{\boldsymbol{\alpha}'}f(\boldsymbol{\psi} + \boldsymbol{h}_\varepsilon(\boldsymbol{\psi}), \boldsymbol{\beta}_0 + \boldsymbol{k}_\varepsilon(\boldsymbol{\psi})) \\ (\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\psi}})^2\boldsymbol{k}_\varepsilon(\boldsymbol{\psi}) &= -\varepsilon\partial_{\boldsymbol{\beta}}f(\boldsymbol{\psi} + \boldsymbol{h}_\varepsilon(\boldsymbol{\psi}) + \boldsymbol{k}_\varepsilon(\boldsymbol{\psi})) \end{aligned} \qquad [89]$$

can be formally solved in powers of ε.

Given the simplicity of the Hamiltonian [80] that we are considering, it is not necessary to discuss the functions $\boldsymbol{H}_\varepsilon, \boldsymbol{K}_\varepsilon$ because the equations that they should obey reduce to their definitions as in the section "Quasiperiodicity and KAM stability," and for the same reason.

In other words, also the resonant tori admit a Lindstedt series representation. It is however very unlikely that the series are, in general, convergent.

Physically, this new aspect is due to the fact that the linearization of the motion near the torus $\mathcal{T}_{\boldsymbol{A}_0,\boldsymbol{\beta}_0}$ introduces oscillatory motions around $\mathcal{T}_{\boldsymbol{A}'_0,\boldsymbol{\beta}_0}$ with frequencies proportional to the square roots of the positive eigenvalues of the matrix $\varepsilon\partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)$: therefore, it is naively expected that it has to be necessary that a Diophantine property be required on the vector $(\boldsymbol{\omega}, \sqrt{\varepsilon\mu_1}, \dots)$, where $\varepsilon\mu_j$ are the positive eigenvalues. Hence, some values of ε, namely those for which $(\boldsymbol{\omega}, \sqrt{\varepsilon\mu_1}, \dots)$ is not a Diophantine vector or is too close to a non-Diophantine vector, should be excluded or at least should be expected to generate difficulties. Note that the problem arises irrespective of the assumptions about the nondegenerate matrix $\partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)$ (since ε can have either sign), and no matter how small $|\varepsilon|$ is supposed to be. But we can expect that if the matrix $\partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)$ is (say) positive definite (i.e., $\boldsymbol{\beta}_0$ is a minimum point for $\bar{f}(\boldsymbol{\beta})$) then the problem should be easier for $\varepsilon < 0$ and vice versa, if $\boldsymbol{\beta}_0$ is a maximum, it should be easier for $\varepsilon > 0$ (i.e., in the cases in which the eigenvalues of $\varepsilon\partial^2_{\boldsymbol{\beta}\boldsymbol{\beta}}\bar{f}(\boldsymbol{\beta}_0)$ are negative and their roots do not have the interpretation of frequencies).

Technically, the sums of the formal series can be given (so far) a meaning only via summation rules involving divergent series: typically, one has to identify in the formal expressions (denumerably many) geometric series which, although divergent, can be given a meaning by applying the rule [79]. Since the rule can only be applied if $z \neq 1$, this leads to conditions on the parameter ε, in order to exclude that the various z that have to be considered are very close to 1. Hence, this stability result turns out to be rather different from the KAM result for the maximal tori. Namely the series can be given a

meaning via summation rules provided f and $\boldsymbol{\beta}_0$ satisfy certain additional conditions and provided certain values of ε are excluded. An example of a theorem is the following:

Theorem 6 *Given the Hamiltonian* [80] *and a resonant torus* $T_{\mathbf{A}'_0,\boldsymbol{\beta}_0}$ *with* $\boldsymbol{\omega}=\mathbf{A}'_0\in\mathbb{R}^r$ *satisfying a Diophantine property let* $\boldsymbol{\beta}_0$ *be a nondegenerate maximum point for the average potential* $\bar{f}(\boldsymbol{\beta})\stackrel{\text{def}}{=}(2\pi)^{-r}\int_{\mathbb{T}^r} f(\boldsymbol{\alpha}',\boldsymbol{\beta})d^r\boldsymbol{\alpha}'$. *Consider the Lindstedt series solution for* eqns [89] *of the perturbed resonant torus with spectrum* $(\boldsymbol{\omega},\mathbf{0})$. *It is possible to express the single nth-order term of the series as a sum of many terms and then rearrange the series thus obtained so that the resummed series converges for* ε *in a domain* $\mathcal{E}$ *which contains a segment* $[0,\varepsilon_0]$ *and also a subset of* $[-\varepsilon_0,0]$ *which, although with open dense complement, is so large that it has* 0 *as a Lebesgue density point. Furthermore, the resummed series for* $\mathbf{h}_\varepsilon,\mathbf{k}_\varepsilon$ *define an invariant r-dimensional analytic torus with spectrum* $\boldsymbol{\omega}$.

More generally, if $\boldsymbol{\beta}_0$ is only a nondegenerate stationarity point for $\bar{f}(\boldsymbol{\beta})$, the domain of definition of the resummed series is a set $\mathcal{E}\subset[-\varepsilon_0,\varepsilon_0]$ which on both sides of the origin has an open dense complement although it has 0 as a Lebesgue density point.

Theorem 6 can be naturally extended to the general case in which the Hamiltonian is the most general perturbation of an anisochronous integrable system $\mathcal{H}_\varepsilon(\mathbf{A},\boldsymbol{\alpha})=h(\mathbf{A})+\varepsilon f(\mathbf{A},\boldsymbol{\alpha})$ if $\partial^2_{\mathbf{AA}}h$ is a nonsingular matrix and the resonance arises from a spectrum $\boldsymbol{\omega}(\mathbf{A}_0)$ which has r independent components (while the remaining are not necessarily zero).

We see that the convergence is a delicate problem for the Lindstedt series for nearly integrable resonant motions. They might even be divergent (mathematically, a proof of divergence is an open problem but it is a very reasonable conjecture in view of the above physical interpretation); nevertheless, Theorem 6 shows that sum rules can be given that sometimes (i.e., for ε in a large set near $\varepsilon=0$) yield a true solution to the problem.

This is reminiscent of the phenomenon met in discussing perturbations of isochronous systems in [76], but it is a much more complex situation. It leaves many open problems: foremost among them is the question of uniqueness. The sum rules of divergent series always contain some arbitrary choices, which lead to doubts about the uniqueness of the functions parametrizing the invariant tori constructed in this way. It might even be that the convergence set $\mathcal{E}$ may depend upon the arbitrary choices, and that considering several of them no ε with $|\varepsilon|<\varepsilon_0$ is left out.

The case of *a priori* unstable systems has also been widely studied. In this case too resonances with Diophantine r-dimensional spectrum $\boldsymbol{\omega}$ are considered. However, in the case $s_2=0$ (called *a priori* unstable hyperbolic resonance) the Lindstedt series can be shown to be convergent, while in the case $s_1=0$ (called *a priori* unstable elliptic resonance) or in the mixed cases $s_1,s_2>0$ extra conditions are needed. They involve $\boldsymbol{\omega}$ and $\boldsymbol{\mu}=(\mu_1,\ldots,\mu_{s_2})$ (cf. [86]) and properties of the perturbations as well. It is also possible to study a slightly different problem: namely to look for conditions on $\boldsymbol{\omega},\boldsymbol{\mu},f$ which imply that, for small ε, invariant tori with spectrum ε-dependent but close, in a suitable sense, to $\boldsymbol{\omega}$ exist.

The literature is vast, but it seems fair to say that, given the above comments, particularly those concerning uniqueness and analyticity, the situation is still quite unsatisfactory. We refer the reader to Gallavotti *et al.* (2004) for more details.

Diffusion in Phase Space

The KAM theorem implies that a perturbation of an analytic anisochronous integrable system, i.e., with an analytic Hamiltonian $\mathcal{H}_\varepsilon(\mathbf{A},\boldsymbol{\alpha})=\mathcal{H}_0(\mathbf{A})+\varepsilon f(\mathbf{A},\boldsymbol{\alpha})$ and nondegenerate Hessian matrix $\partial^2_{\mathbf{AA}}h(\mathbf{A})$, generates large families of maximal invariant tori. Such tori lie on the energy surfaces but do not have codimension 1 on them, i.e., they do not split the $(2\ell-1)$–dimensional energy surfaces into disconnected regions except, of course, in the case of systems with two degrees of freedom (see the section "Quasiperiodicity and KAM stability").

Therefore, there might exist trajectories with initial data close to $\mathbf{A}^{\mathrm{i}}$ in action space which reach phase space points close to $\mathbf{A}^{\mathrm{f}}\neq\mathbf{A}^{\mathrm{i}}$ in action space for $\varepsilon\neq0$, *no matter how small*. Such *diffusion* phenomenon would occur in spite of the fact that the corresponding trajectory has to move in a space in which very close to each $\{\mathbf{A}\}\times\mathbb{T}^\ell$ there is an invariant surface on which points move keeping $\mathbf{A}$ constant within $O(\varepsilon)$, which for ε small can be $\ll|\mathbf{A}^{\mathrm{f}}-\mathbf{A}^{\mathrm{i}}|$.

In *a priori* unstable systems (cf. the section "Resonances and their stability") with $s_1=1$, $s_2=0$, it is not difficult to see that the corresponding phenomenon can actually occur: the paradigmatic example (Arnol'd) is the *a priori* unstable system

$$\mathcal{H}_\varepsilon=\frac{A_1^2}{2}+A_2+\frac{p^2}{2}+g(\cos q-1)+\varepsilon(\cos\alpha_1+\sin\alpha_2)(\cos q-1)\qquad[90]$$

This is a system describing a motion of a "pendulum" ((p, q) coordinates) interacting with a "rotating wheel" ((A_1, α_1) coordinates) and a "clock" ((A_2, α_2) coordinates) *a priori* unstable near the points $p = 0, q = 0, 2\pi$ ($s_1 = 1, s_2 = 0, \lambda_1 = \sqrt{g}$, cf. [86]). It can be proved that on the energy surface of energy E and for each $\varepsilon \neq 0$ small enough (no matter how small) there are initial data with action coordinates close to $A^i = (A_1^i, A_2^i)$ with $(1/2)A_1^{i2} + A_2^i$ close to E eventually evolving to a datum $A' = (A_1', A_2')$ with A_1' at a distance from A_1^f smaller than an arbitrarily prefixed distance (of course with energy E). Furthermore, during the whole process the pendulum energy stays close to zero within $o(\varepsilon)$ (i.e., the pendulum swings following closely the unperturbed separatrices).

In other words, [90] describes a machine (the pendulum) which, working approximately in a cycle, extracts energy from a reservoir (the clock) to transfer it to a mechanical device (the wheel). The statement that diffusion is possible means that the machine can work as soon as $\varepsilon \neq 0$, if the initial actions and the initial phases (i.e., α_1, α_2, p, q) are suitably tuned (as functions of ε).

The peculiarity of the system [90] is that the fixed points $P_\pm$ of the unperturbed pendulum (i.e., the equilibria $p = 0, q = 0, 2\pi$) *remain* unstable equilibria even when $\varepsilon \neq 0$ and this is an important simplifying feature.

It is a peculiarity that permits bypassing the obstacle, arising in the analysis of more general cases, represented by the resonance surfaces consisting of the A's with $A_1\nu_1 + \nu_2 = 0$: the latter correspond to harmonics (ν_1, ν_2) present in the perturbing function, i.e., the harmonics which would lead to division by zero in an attempt to construct (as necessary in studying [90] by Arnol'd's method) the parametric equations of the perturbed invariant tori with action close to such A's. In the case of [90] the problem arises only on the resonance marked in **Figure 6** by a heavy line, i.e., $A_1 = 0$, corresponding to $\cos\alpha_1$ in [90].

If $\varepsilon = 0$, the points P_- with $p = 0, q = 0$ and the point P_+ with $p = 0, q = 2\pi$ are both unstable equilibria (and they are, of course, the same point, if q is an angular variable). The unstable manifold (it is a curve) of P_+ coincides with the stable manifold of P_- and vice versa. So that the unperturbed system admits nontrivial motions leading from P_+ to P_- and from P_- to P_+, both in a bi-infinite time interval $(-\infty, \infty)$: the p, q variables describe a pendulum and $P_\pm$ are its unstable equilibria which are connected by the separatrices (which constitute the zero-energy surfaces for the pendulum).

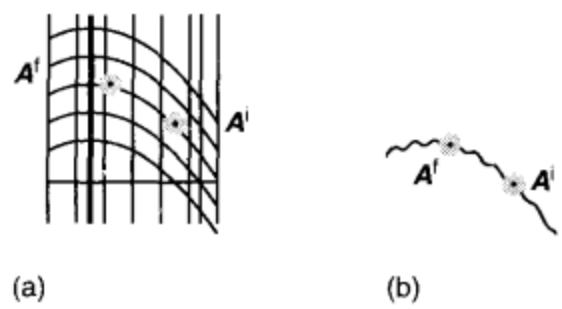

Figure 6 (a) The $\varepsilon = 0$ geometry: the "partial energy" lines are parabolas, $(1/2)A_1^2 + A_2 = \text{const}$. The vertical lines are the resonances $A_1 = \text{rational}$ (i.e., $\nu_1 A_1 + \nu_2 = 0$). The disks are neighborhoods of the points $\boldsymbol{A}^i$ and $\boldsymbol{A}^f$ (the dots at their centers). (b) $\varepsilon \neq 0$; an artist's rendering of a trajectory in $\boldsymbol{A}$ space, driven by the pendulum swings to accelerate the wheel from A_1^i to A_1^f at the expenses of the clock energy, sneaking through invariant tori not represented and (approximately) located "away" from the intersections between resonances and partial energy lines (a dense set, however). The pendulum coordinates are not shown: its energy stays close to zero, within a power of ε. Hence the pendulum swings, staying close to the separatrix. The oscillations symbolize the wiggly behavior of the partial energy $(1/2)A_1^2 + A_2$ in the process of sneaking between invariant tori which, because of their invariance, would be impossible without the pendulum. The energy $(1/2)A_1^2$ of the wheel increases slightly at each pendulum swing: accurate estimates yield an increase of the wheel speed A_1 of the order of $\varepsilon/(\log \varepsilon^{-1})$ at each swing of the pendulum implying a transition time of the order of $g^{-1/2}\varepsilon^{-1}\log\varepsilon^{-1}$.

The latter property remains true for more general *a priori* unstable Hamiltonians

$$\mathcal{H}_\varepsilon = \mathcal{H}_0(\boldsymbol{A}) + \mathcal{H}_u(p, q) + \varepsilon f(\boldsymbol{A}, \boldsymbol{\alpha}, p, q) \quad \text{in } (U \times \mathbb{T}^\ell) \times (\mathbb{R}^2) \qquad [91]$$

where $\mathcal{H}_u$ is a one-dimensional Hamiltonian which has two unstable equilibrium points P_+ and P_- linearly repulsive in one direction and linearly attractive in another which are connected by two heteroclinic trajectories which, as time tends to $\pm\infty$, approach P_- and P_+ and vice versa.

Actually, the points need not be different but, if coinciding, the trajectories linking them must be nontrivial: in the case [90] the variable q can be considered an angle and then P_+ and P_- would coincide (but are connected by nontrivial trajectories, i.e., by trajectories that also visit points different from $P_\pm$). Such trajectories are called heteroclinic if $P_+ \neq P_-$ and homoclinic if $P_+ = P_-$.

In the general case, besides the homoclinicity (or heteroclinicity) condition, certain weak genericity conditions, automatically satisfied in the example [90], have to be imposed in order to show that, given A^i and A^f with the same unperturbed energy E, one can find, for all ε small enough but not equal to zero, initial data (ε-dependent) with actions arbitrarily close to A^i which evolve to data with actions arbitrarily close to A^f. This is a phenomenon

called the *Arnol'd diffusion*. Simple sufficient conditions for a transition from near A^i to near A^f are expressed by the following result:

Theorem 7 *Given the Hamiltonian* [91] *with* $\mathcal{H}_u$ *admitting two hyperbolic fixed points* $P_\pm$ *with heteroclinic connections,* $t \to (p_a(t), q_a(t))$, $a = 1, 2$, *suppose that*:

(i) *On the unperturbed energy surface of energy* $E = \mathcal{H}(A^i) + \mathcal{H}_u(P_\pm)$ *there is a regular curve* $\gamma : s \to A(s)$ *joining* A^i *to* A^f *such that the unperturbed tori* $\{A(s)\} \times \mathbb{T}^\ell$ *can be continued at* $\varepsilon \neq 0$ *into invariant tori* $\mathcal{T}_{A(s),\varepsilon}$ *for a set of values of* s *which fills the curve* γ *leaving only gaps of size of order* $o(\varepsilon)$.

(ii) *The* $\ell \times \ell$ *matrix* D_{ij} *of the second derivatives of the integral of* f *over the heteroclinic motions is not degenerate, that is,*

$$|\det D| = \left| \det \left(\int_{-\infty}^{\infty} dt\, \partial_{\alpha_i \alpha_j} f(A, \alpha + \omega(A)t, p_a(t), q_a(t)) \right) \right| > c > 0 \qquad [92]$$

for all A*'s on the curve* γ *and all* $\alpha \in \mathbb{T}^2$.

Given arbitrary $\rho > 0$, *for* $\varepsilon \neq 0$ *small enough there are initial data with action and energy closer than* ρ *to* A^i *and* E, *respectively, which after a long enough time acquire an action closer than* ρ *to* A^f (*keeping the initial energy*).

The above two conditions can be shown to hold generically for many pairs $A^i \neq A^f$ (and many choices of the curves γ connecting them) if the number of degrees of freedom is ≥ 3. Thus, the result, obtained by a simple extension of the argument originally outlined by Arnol'd to discuss the paradigmatic example [90], proves the existence of diffusion in *a priori* unstable systems. The integral in [92] is called *Melnikov integral*.

The real difficulty is to estimate the time needed for the transition: it is a time that obviously has to diverge as $\varepsilon \to 0$. Assuming g fixed (i.e., ε independent) a naive approach easily leads to estimates which can even be worse than $O(\exp(a\varepsilon^{-b}))$ with some $a, b > 0$. It has finally been shown that in such cases the minimum time can be, for rather general perturbations $\varepsilon f(\alpha, q)$, estimated above by $O(\varepsilon^{-1} \log \varepsilon^{-1})$, which is the best that can be hoped for under generic assumptions.

The reader is referred to Arnol'd (1989) and Chierchia and Valdinoci (2000) for more details.

Long-Time Stability of Quasiperiodic Motions

A more difficult problem is whether the same phenomenon of migration in action space occurs in *a priori* stable systems. The root of the difficulty is a remarkable stability property of quasiperiodic motions. Consider Hamiltonians $\mathcal{H}_\varepsilon(A, \alpha) = h(A) + \varepsilon f(A, \alpha)$ with $\mathcal{H}_0(A) = h(A)$ strictly convex, analytic, and anisochronous on the closure $\overline{U}$ of an open bounded region $U \subset \mathbb{R}^\ell$, and a perturbation $\varepsilon f(A, \alpha)$ analytic in $\overline{U} \times \mathbb{T}^\ell$.

Then *a priori* bounds are available on how long it can possibly take to migrate from an action close to A_1 to one close to A_2: and the bound is of "exponential type" as $\varepsilon \to 0$ (i.e., it admits a lower bound which behaves as the exponential of an inverse power of ε). The simplest theorem is (Nekhorossev):

Theorem 7 *There are constants* $0 < a, b, d, g, \tau$ *such that any initial datum* (A, α) *evolves so that* A *will not change by more than* $a\varepsilon^g$ *before a long time bounded below by* $\tau \exp(b\varepsilon^{-d})$.

Thus, this puts an exponential bound, i.e., a bound exponential in an inverse power of ε, to the diffusion time: before a time $\tau \exp(b\varepsilon^{-d})$ actions can only change by $O(\varepsilon^g)$ so that their variation cannot be large no matter how small $\varepsilon \neq 0$ is chosen. This places a (long) lower bound to the time of diffusion in *a priori* stable systems.

The proof of the theorem provides, actually, an interesting and detailed picture of the variations in actions showing that some actions may vary more slowly than others.

The theorem is constructive, i.e., all constants $0 < a, b, d, \tau$ can be explicitly chosen and depend on $\ell, \mathcal{H}_0, f$ although some of them can be fixed to depend only on ℓ and on the minimum curvature of the convex graph of $\mathcal{H}_0$. Its proof can be adapted to cover many cases which do not fall in the class of systems with strictly convex unperturbed Hamiltonian, and even to cases with a resonant unperturbed Hamiltonian.

However, in important problems (e.g., in the three-body problems met in celestial mechanics) there is empirical evidence that diffusion takes place at a fast pace (i.e., not exponentially slow in the above sense) while the above results would forbid a rapid migration in phase space if they applied: however, in such problems the assumptions of the theorem are not satisfied, because the unperturbed system is strongly resonant (as in the celestial mechanics problems, where the number of independent frequencies is a fraction of the number

of degrees of freedom and $h(A)$ is far from strictly convex), leaving wide open the possibility of observing rapid diffusion.

Further, changing the assumptions can dramatically change the results. For instance, rapid diffusion can sometimes be proved even though it might be feared that it should require exponentially long times: an example that has been proposed is the case of a three-timescales system, with Hamiltonian

$$\omega_1 A_1 + \omega_2 A_2 + \frac{p^2}{2} + g(1+\cos q) + \varepsilon f(\alpha_1, \alpha_2, p, q) \qquad [93]$$

with $\boldsymbol{\omega}_\varepsilon \stackrel{\text{def}}{=} (\omega_1, \omega_2)$, where $\omega_1 = \varepsilon^{-1/2}\overline{\omega}$, $\omega_2 = \varepsilon^{1/2}\widetilde{\omega}$ and $\overline{\omega}, \widetilde{\omega} > 0$ constants. The three scales are ω_1^{-1}, $\sqrt{g^{-1}}$, ω_2^{-1}. In this case, there are many (although by no means all) pairs A_1, A_2 which can be connected within a time that can be estimated to be of order $O(\varepsilon^{-1}\log\varepsilon^{-1})$.

This is a rapid-diffusion case in an *a priori* unstable system in which condition [92] is not satisfied: because the ε-dependence of $\boldsymbol{\omega}(A)$ implies that the lower bound c in [92] must depend on ε (and be exponentially small with an inverse power of ε as $\varepsilon \to 0$).

The unperturbed system in [93] is nonresonant in the $\mathcal{H}_0$ part for $\varepsilon > 0$ outside a set of zero measure (i.e., where the vector $\boldsymbol{\omega}_\varepsilon$ satisfies a suitable Diophantine property) and, furthermore, it is *a priori* unstable: cases met in applications can be *a priori* stable and resonant (and often not anisochronous) in the $\mathcal{H}_0$ part. In such a system, not only the speed of diffusion is not understood but proposals to prove its existence, if present (as expected), have so far not given really satisfactory results.

For more details, the reader in referred to Nekhorossev (1977).

The Three-Body Problem

Mechanics and the three-body problem can be almost identified with each other, in the sense that the motion of three gravitating masses has long been a key astronomical problem and at the same time the source of inspiration for many techniques: foremost among them the theory of perturbations.

As an introduction, consider a special case. Let three masses $m_S = m_0$, $m_J = m_1$, $m_M = m_2$ interact via gravity, that is, with interaction potential $-km_i m_j |\boldsymbol{x}_i - \boldsymbol{x}_j|^{-1}$: the simplest problem arises when the third body has a neglegible mass compared to the two others and the latter are supposed to be on a circular orbit; furthermore, the mass m_J is εm_S with ε small and the mass m_M moves in the plane of the circular orbit. This will be called the "circular restricted three-body problem."

In a reference system with center S and rotating at the angular speed of J around S inertial forces (centrifugal and Coriolis) act. Supposing that the body J is located on the axis with unit vector $\boldsymbol{i}$ at distance R from the origin S, the acceleration of the point M is

$$\ddot{\varrho} = \boldsymbol{F} + \omega_0^2\left(\varrho - \frac{\varepsilon R}{1+\varepsilon}\boldsymbol{i}\right) - 2\boldsymbol{\omega}_0 \wedge \dot{\varrho}$$

if $\boldsymbol{F}$ is the force of attraction and $\boldsymbol{\omega}_0 \wedge \dot{\varrho} \equiv \omega_0 \dot{\varrho}^\perp$ where $\boldsymbol{\omega}_0$ is a vector with $|\boldsymbol{\omega}_0| = \omega_0$ and perpendicular to the orbital plane and $\varrho^\perp \stackrel{\text{def}}{=} (-\rho_2, \rho_1)$ if $\varrho = (\rho_1, \rho_2)$. Here, taking into account that the origin S rotates around the fixed center of mass, $\omega_0^2(\varrho - \varepsilon R/(1+\varepsilon)\boldsymbol{i})$ is the centrifugal force while $-2\boldsymbol{\omega}_0 \wedge \dot{\varrho}$ is the Coriolis force. The equations of motion can therefore be derived from a Lagrangian

$$\mathcal{L} = \frac{1}{2}\dot{\varrho}^2 - W + \omega_0 \varrho^\perp \cdot \dot{\varrho} + \frac{1}{2}\omega_0^2 \varrho^2 - \omega_0^2 \frac{\varepsilon R}{1+\varepsilon}\varrho \cdot \boldsymbol{i} \qquad [94]$$

with

$$\omega_0^2 R^3 = km_S(1+\varepsilon) \stackrel{\text{def}}{=} g_0$$
$$W = -\frac{km_S}{|\varrho|} - \frac{km_S\varepsilon}{|\varrho - R\boldsymbol{i}|}$$

where k is the gravitational constant, R the distance between S and J, and finally the last three terms in [94] come from the Coriolis force (the first) and from the centripetal force (the other two, taking into account that the origin S rotates around the fixed center of mass).

Setting $g = g_0/(1+\varepsilon) \equiv km_S$, the Hamiltonian of the system is

$$\mathcal{H} = \frac{1}{2}(\boldsymbol{p} - \omega_0 \varrho^\perp)^2 - \frac{g}{|\varrho|} - \frac{1}{2}\omega_0^2 \varrho^2 - \varepsilon\frac{g}{R}\left(\left|\frac{\varrho}{R} - \boldsymbol{i}\right|^{-1} - \frac{\varrho}{R}\cdot\boldsymbol{i}\right) \qquad [95]$$

The first part can be expressed immediately in the action–angle coordinates for the two-body problem (cf. the section "Newtonian potential and Kepler's laws"). Calling such coordinates $(L_0, \lambda_0, G_0, \gamma_0)$ and θ_0 the polar angle of M with respect to the major axis of the ellipse and λ_0 the mean anomaly of M on its ellipse, the Hamiltonian becomes, taking into account that for $\varepsilon = 0$ the ellipse axis rotates at speed $-\omega_0$,

$$\mathcal{H} = -\frac{g^2}{2L_0^2} - \omega_0 G_0 - \varepsilon\frac{g}{R}\left(\left|\frac{\varrho}{R} - \boldsymbol{i}\right|^{-1} - \frac{\varrho}{R}\cdot\boldsymbol{i}\right) \qquad [96]$$

which is convenient if we study the interior problem, i.e., $|\varrho| < R$. This can be expressed in the action–angle coordinates via [41], [42]:

$$\theta_0 = \lambda_0 + f_{\lambda_0}, \qquad \theta_0 + \gamma_0 = \lambda_0 + \gamma_0 + f_{\lambda_0}$$
$$e = \left(1 - \frac{G_0^2}{L_0^2}\right)^{1/2}, \quad \frac{|\varrho|}{R} = \frac{G_0^2}{gR}\frac{1}{1 + e\cos(\lambda_0 + f_{\lambda_0})} \qquad [97]$$

where (see [42]), $f_\lambda = f(e\sin\lambda, e\cos\lambda)$ and

$$f(x,y) = 2x\left(1 + \frac{5}{4}y + \cdots\right)$$

with the ellipsis denoting higher orders in x, y even in x. The Hamiltonian takes the form, if $\omega^2 = gR^{-3}$,

$$\mathcal{H}_\varepsilon = -\frac{g^2}{2L_0^2} - \omega G_0 + \varepsilon\frac{g}{R}F(G_0, L_0, \lambda_0, \lambda_0 + \gamma_0) \qquad [98]$$

where the only important feature (for our purposes) is that $F(L, G, \alpha, \beta)$ is an analytic function of L, G, α, β near a datum with $|G| < L$ (i.e., $e > 0$) and $|\varrho| < R$. However, the domain of analyticity in G is rather small as it is constrained by $|G| < L$ excluding in particular the circular orbit case $G = \pm L$.

Note that apparently the KAM theorem fails to be applicable to [98] because the matrix of the second derivatives of $\mathcal{H}_0(L, G)$ has vanishing determinant. Nevertheless, the proof of the theorem also goes through in this case, with minor changes. This can be checked by studying the proof or, following a remark by Poincaré, by simply noting that the "squared" Hamiltonian $\mathcal{H}'_\varepsilon \stackrel{\text{def}}{=} (\mathcal{H}_\varepsilon)^2$ has the form

$$\mathcal{H}'_\varepsilon = \left(-\frac{g^2}{2L_0^2} - \omega G_0\right)^2 + \varepsilon F'(G_0, L_0, \lambda_0, \lambda_0 + \gamma_0) \qquad [99]$$

with F' still analytic. *But* this time

$$\det\frac{\partial^2 \mathcal{H}'_0}{\partial(G_0, L_0)} = -6g^2 L_0^{-4}\omega_0^2 h \neq 0$$
$$\text{if } h = -g^2 L_0^{-2} - 2\omega G_0 \neq 0$$

Therefore, the KAM theorem applies to $\mathcal{H}'_\varepsilon$ and the key observation is that the orbits generated by the Hamiltonian $(\mathcal{H}_\varepsilon)^2$ are geometrically the same as those generated by the Hamiltonian $\mathcal{H}_\varepsilon$: they are only run at a different speed because of the need of a time rescaling by the constant factor $2\mathcal{H}_\varepsilon$.

This shows that, given an unperturbed ellipse of parameters (L_0, G_0) such that $\boldsymbol{\omega} = (g^2/L_0^3, -\omega)$, $G_0 > 0$, with ω_1/ω_2 Diophantine, then the perturbed system admits a motion which is quasiperiodic with spectrum proportional to $\boldsymbol{\omega}$ and takes place on an orbit which wraps around a torus remaining forever close to the unperturbed torus (which can be visualized as described by a point moving, according to the area law on an ellipse rotating at a rate $-\omega_0$) with actions (L_0, G_0), provided ε is small enough. Hence,

> The KAM theorem answers, at least conceptually, the classical question: can a solution of the three-body problem remain close to an unperturbed one forever? That is, is it possible that a solar system is stable forever?

Assuming $e, |\varrho|/R \ll 1$ and retaining only the lowest orders in e and $|\varrho|/R \ll 1$ the Hamiltonian [98] simplifies into

$$\mathcal{H} = -\frac{g^2}{2L_0^2} - \omega G_0 + \delta_\varepsilon(G_0) - \frac{\varepsilon g}{2R}\frac{G_0^4}{g^2R^2}\left(3\cos 2(\lambda_0 + \gamma_0) - e\cos\lambda_0 - \frac{9}{2}e\cos(\lambda_0 + 2\gamma_0) + \frac{3}{2}e\cos(3\lambda_0 + 2\gamma_0)\right) \qquad [100]$$

where

$$\delta_\varepsilon(G_0) = -((1+\varepsilon)^{1/2} - 1)\omega G_0 - \frac{\varepsilon g}{2R}\frac{G_0^4}{g^2R^2}$$
$$e = \left(1 - \frac{G_0^2}{L_0^2}\right)^{1/2}$$

It is an interesting exercise to estimate, assuming as model the Hamiltonian [100] and following the proof of the KAM theorem, how small has ε to be if a planet with the data of Mercury can be stable forever on a (slowly precessing) orbit with actions close to the present-day values under the influence of a mass ε times the solar mass orbiting on a circle, at a distance from the Sun equal to that of Jupiter. It is possible to follow either the above reduction to the ordinary KAM theorem or to apply directly to [100] the Lindstedt series expansion, proceeding along the lines of the section "Quasiperiodicity and KAM stability." The first approach is easy but the second is more efficient: in both cases, unless the estimates are done in a particularly careful manner, the value found for εm_S is not interesting from the viewpoint of astronomy.

The reader is refered to Arnol'd (1989) for more details.

Rationalization and Regularization of Singularities

Often integrable systems have interesting data which lie on the boundary of the integrability domain. For instance, the central motion when $L = G$ (circular orbits) or the rigid body in a rotation around one of the principal axes or the two-body problem when $G = 0$ (collisional data). In such cases, perturbation

theory cannot be applied as discussed above. Typically, the perturbation depends on quantities like $\sqrt{L-G}$ and is *not analytic* at $L=G$. Nevertheless, it is sometimes possible to enlarge phase space and introduce new coordinates in the vicinity of the data which in the initial phase space are singular.

A notable example is the failure of the analysis of the circular restricted three-body problem: it apparently fails when the orbit that we want to perturb is circular.

It is convenient to introduce the canonical coordinates L, λ and G, γ:

$$\begin{aligned} L &= L_0, \qquad G = L_0 - G_0 \\ \lambda &= \lambda_0 + \gamma_0, \qquad \gamma = -\gamma_0 \end{aligned} \tag{101}$$

so that $e = \sqrt{2GL^{-1}}\sqrt{1 - G(2L)^{-1}}$ and $\lambda_0 = \lambda + \gamma$ and $\theta_0 = \lambda_0 + f_{\lambda_0}$, where f_{λ_0} is defined in [42] (see also [97]). Hence,

$$\begin{aligned} &\theta_0 = \lambda + \gamma + f_{\lambda+\gamma}, \qquad \theta_0 + \gamma_0 = \lambda + f_{\lambda+\gamma} \\ &e = \sqrt{2G}\sqrt{\frac{1}{L}\left(1 - \frac{G}{2L}\right)} \\ &\frac{|\varrho|}{R} = \frac{L^2(1-e^2)}{gR}\,\frac{1}{1 + e\cos(\lambda + \gamma + f_{\lambda+\gamma})} \end{aligned} \tag{102}$$

and the Hamiltonian [100] takes the form

$$\begin{aligned} \mathcal{H}_\varepsilon = &-\frac{g^2}{2L^2} - \omega L + \omega G \\ &+ \varepsilon \frac{g}{R} F(L - G, L, \lambda + \gamma, \lambda) \end{aligned} \tag{103}$$

In the coordinates L,G of [101] the unperturbed circular case corresponds to $G=0$ and [96], once expressed in the action–angle variables G, L, γ, λ, is analytic in a domain whose size is controlled by $\sqrt{G}$. Nevertheless, very often problems of perturbation theory can be "regularized."

This is done by "enlarging the integrability" domain by adding to it points (one or more) around the singularity (a boundary point of the domain of the coordinates) and introducing new coordinates to describe simultaneously the data close to the singularity and the newly added points: in many interesting cases, the equations of motion are no longer singular (i.e., become analytic) in the new coordinates and are therefore apt to describe the motions that reach the singularity in a finite time. One can say that the singularity was only apparent.

Perhaps this is best illustrated precisely in the above circular restricted three-body problem, with the singularity occurring where $G=0$, that is, at a circular unperturbed orbit. If we describe the points with G small in a new system of coordinates obtained from the one in [101] by letting alone L, λ and setting

$$p = \sqrt{2G}\cos\gamma, \qquad q = \sqrt{2G}\sin\gamma \tag{104}$$

then p, q vary in a neighborhood of the origin with the origin itself excluded.

Adding the origin of the p–q plane then in a full neighborhood of the origin, the Hamiltonian [96] is analytic in L, λ, p, q. This is because it is analytic (cf. [96], [97]) as a function of L, λ and $e\cos\theta_0$ and of $\cos(\lambda_0 + \theta_0)$. Since $\theta_0 = \lambda + \gamma + f_{\lambda+\gamma}$ and $\theta_0 + \lambda_0 = \lambda + f_{\lambda+\gamma}$ by [97], the Hamiltonian [96] is analytic in $L, \lambda, e\cos(\lambda + \gamma + f_{\lambda+\gamma}), \cos(\lambda + f_{\lambda+\gamma})$ for e small (i.e., for G small) and, by [42], $f_{\lambda+\gamma}$ is analytic in $e\sin(\lambda+\gamma)$ and $e\cos(\lambda+\gamma)$. Hence the trigonometric identities

$$\begin{aligned} e\sin(\lambda+\gamma) &= \frac{p\sin\lambda + q\cos\lambda}{\sqrt{L}}\sqrt{1 - \frac{G}{2L}} \\ e\cos(\lambda+\gamma) &= \frac{p\cos\lambda - q\sin\lambda}{\sqrt{L}}\sqrt{1 - \frac{G}{2L}} \end{aligned} \tag{105}$$

together with $G = (1/2)(p^2 + q^2)$ imply that [103] is analytic near $p=q=0$ and $L>0, \lambda \in [0, 2\pi]$. The Hamiltonian becomes analytic and the new coordinates are suitable to describe motions crossing the origin: for example, by setting

$$C \overset{\text{def}}{=} \frac{1}{2}\left(1 - \frac{p^2+q^2}{4L}\right)L^{-1/2}$$

[100] becomes

$$\begin{aligned} \mathcal{H} = &-\frac{g^2}{2L^2} - \omega L + \omega\tfrac{1}{2}(p^2+q^2) \\ &+ \delta_\varepsilon(\tfrac{1}{2}(p^2+q^2)) - \frac{\varepsilon g}{2R}\frac{(L - \frac{1}{2}(p^2+q^2))^4}{g^2R^2} \\ &\times (3\cos 2\lambda - ((-11\cos\lambda + 3\cos 3\lambda)p \\ &- (7\sin\lambda + 3\sin 3\lambda)q)C) \end{aligned} \tag{106}$$

The KAM theorem does not apply in the form discussed above to "Cartesian coordinates," that is, when, as in [106], the unperturbed system is not assigned in action–angle variables. However, there are versions of the theorem (actually its corollaries) which do apply and therefore it becomes possible to obtain some results even for the perturbations of circular motions by the techniques that have been illustrated here.

Likewise, the Hamiltonian of the rigid body with a fixed point O and subject to analytic external forces becomes singular, if expressed in the action–angle coordinates of Deprit, when the body motion nears a rotation around a principal axis or, more generally, nears a configuration in which any two of

the axes i_3, z, or z_0 coincide (i.e., any two among the principal axis, the angular momentum axis and the inertial z-axis coincide; see the section "Rigid body"). Nevertheless, by imitating the procedure just described in the simpler cases of the circular three-body problem, it is possible to enlarge the phase space so that in the new coordinates the Hamiltonian is analytic near the singular configurations.

A regularization also arises when considering collisional orbits in the unrestricted planar three-body problem. In this respect, a very remarkable result is the regularization of collisional orbits in the planar three-body problem. After proving that if the total angular momentum does not vanish, simultaneous collisions of the three masses cannot occur within any finite time interval, the question is reduced to the regularization of two-body collisions, under the assumption that the total angular momentum does not vanish.

The local change of coordinates, which changes the relative position coordinates (x, y) of two colliding bodies as $(x, y) \to (\xi, \eta)$, with $x + iy = (\xi + i\eta)^2$, is not one to one, hence it has to be regarded as an enlargement of the positions space, if points with different (ξ, η) are considered different. However, the equations of motion written in the variables ξ, η have no singularity at $\xi, \eta = 0$ (LEVI-CIVITA).

Another celebrated regularization is the regularization of the Schwartzschild metric, i.e., of the general relativity version of the two-body problem: it is, however, somewhat out of the scope of this review (SYNGE, KRUSKAL).

For more details, the reader is refered to Levi-Civita (1956).

Appendix 1: KAM Resummation Scheme

The idea to control the "remaining contributions" is to reduce the problem to the case in which there are no pairs of lines that follow each other in the tree order and which have the same current. Mark by a scale label "0" the lines, see [74], [83], of a tree whose divisors $C/\boldsymbol{\omega}_0.\boldsymbol{\nu}(l)$ are >1: these are lines which give no problems in the estimates. Then mark by a scale label "≥ 1" the lines with current $\boldsymbol{\nu}(l)$ such that $|\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}(l)| \leq 2^{-n+1}$ for $n = 1$ (i.e., the remaining lines).

The lines labeled 0 are said to be on scale 0, while those labeled ≥ 1 are said to be on scale ≥ 1. A cluster of scale 0 will be a maximal collection of lines of scale 0 forming a connected subgraph of a tree θ.

Consider only trees $\theta_0 \in \Theta_0$ of the family Θ_0 of trees containing no clusters of lines with scale label 0 which have only one line entering the cluster and one exiting it with equal current.

It is useful to introduce the notion of a line ℓ_1 situated "between" two lines ℓ, ℓ' with $\ell' > \ell$: this will mean that ℓ_1 precedes ℓ' but not ℓ.

All trees θ in which there are some pairs $l' > l$ of consecutive lines of scale label ≥ 1 which have equal current and such that all lines between them bear scale label 0 are obtained by "inserting" on the lines of trees in Θ_0 with label ≥ 1 any number of clusters of lines and nodes, with lines of scale 0 and with the property that the sum of the harmonics of the nodes inserted vanishes.

Consider a line $l_0 \in \theta_0 \in \Theta_0$ linking nodes $v_1 < v_2$ and labeled ≥ 1 and imagine inserting on it a cluster γ of lines of scale 0 with sum of the node harmonics vanishing and out of which emerges one line connecting a node v_{out} in γ to v_2 and into which enters one line linking v_1 to a node $v_{\text{in}} \in \gamma$. The insertion of a k–lines, $|\gamma| = (k+1)$-nodes, cluster changes the tree value by replacing the line factor, that will be briefly called "value of the cluster γ", as

$$\frac{\boldsymbol{\nu}_{v_1} \cdot \boldsymbol{\nu}_{v_2}}{\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}(l_0)^2} \to \frac{(\boldsymbol{\nu}_{v_1} \cdot M(\gamma; \boldsymbol{\nu}(l_0))\boldsymbol{\nu}_{v_2})}{\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}(l_0)^2} \frac{1}{\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}(l_0)^2} \quad [107]$$

where M is an $\ell \times \ell$ matrix

$$M_{rs}(\gamma, \boldsymbol{\nu}(l_0)) = \frac{\varepsilon^{|\gamma|}}{k!} \nu_{out,r} \nu_{in,s} \prod_{v \in \gamma} (-f_{\nu_v}) \prod_{l \in \gamma} \frac{\boldsymbol{\nu}_v \cdot \boldsymbol{\nu}_{v'}}{\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}(l)^2}$$

if $\ell = v'v$ denotes a line linking v' and v. Therefore, if all possible connected clusters are inserted and the resulting values are added up, the result can be taken into account by attributing to the original line l_0 a factor like [107] with $M^{(0)}(\boldsymbol{\nu}(l_0)) \stackrel{\text{def}}{=} \sum_\gamma M(\gamma; \boldsymbol{\nu}(l_0))$ replacing $M(\gamma; \boldsymbol{\nu}(l_0))$.

If several connected clusters γ are inserted on the same line and their values are summed, the result is a modification of the factor associated with the line l_0 into

$$\sum_{k=0}^{\infty} \boldsymbol{\nu}_{v_1} \cdot \left(\frac{M^{(0)}(\boldsymbol{\nu}(l_0))}{\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}(l_0)^2} \right)^k \boldsymbol{\nu}_{v_2} \frac{1}{\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}(l_0)^2}$$
$$= \left(\boldsymbol{\nu}_{v_1} \cdot \frac{1}{\boldsymbol{\omega}_0 \cdot \boldsymbol{\nu}(l_0)^2 - M^{(0)}(\boldsymbol{\nu}(l_0))} \boldsymbol{\nu}_{v_2} \right) \quad [108]$$

The series defining $M^{(0)}$ involves, by construction, only trees with lines of scale 0, hence with large divisors, so that it converges to a matrix of small size of order ε (actually ε^2, more precisely) if ε is small enough.

Convergence can be established by simply remarking that the series defining $M^{(1)}$ is built with lines with values $>(1/2)$ of the propagator, so that it certainly converges for ε small enough (by the estimates in the section "Perturbing functions," where the propagators were identically 1) and the

sum is of order ε (actually ε^2), hence <1. However, such an argument cannot be repeated when dealing with lines with smaller propagators (which still have to be discussed). Therefore, a method not relying on so trivial a remark on the size of the propagators has eventually to be used when considering lines of scale higher than 1, as it will soon become necessary.

The advantage of the collection of terms achieved with [108] is that we can represent h as a sum of values of trees which are simpler because they contain no pair of lines of scale ≥ 1 with in between lines of scale 0 with total sum of the node harmonics vanishing. The price is that the divisors are now more involved and we even have a problem due to the fact that we have not proved that the series in [108] converges. In fact, it is a geometric series whose value is the RHS of [108] obtained by the sum rule [79] unless we can prove that the ratio of the geometric series is <1. This is trivial in this case by the previous remark: but it is better to note that there is another reason for convergence, whose use is not really necessary here but will become essential later.

The property that the ratio of the geometric series is <1 can be regarded as due to the consequence of the cancellation mentioned in the section "Quasiperiodicity and KAM stability" which can be shown to imply that the ratio is <1 because $M^{(0)}(\nu) = \varepsilon^2(\omega_0 \cdot \nu)^2 m^{(0)}(\nu)$ with $C\,|m^{(0)}(\nu)| < D_0$ for some $D_0 > 0$ and for all $|\varepsilon| < \varepsilon_0$ for some ε_0. Then for small ε the divisor in [108] is essentially still what it was before starting the resummation.

At this point, an induction can be started. Consider trees evaluated with the new rule and place a scale level "≥ 2" on the lines with $C\,|\omega_0 \cdot \nu(l)| \leq 2^{-n+1}$ for $n = 2$: leave the label "0" on the lines already marked so and label by "1" the other lines. The lines of scale "1" will satisfy $2^{-n} < |\omega_0 \cdot \nu(l)| \leq 2^{-n+1}$ for $n = 1$. The graphs will now possibly contain lines of scale 0, 1 or ≥ 2 while lines with label "≥ 1" no longer can appear, by construction.

A cluster of scale 1 will be a maximal collection of lines of scales 0, 1 forming a connected subgraph of a tree θ and containing at least one line of scale 1.

The construction carried out by considering clusters of scale 0 can be repeated by considering trees $\theta_1 \in \Theta_1$, with Θ_1 the collection of trees with lines marked 0, 1, or ≥ 2 and in which no pairs of lines with equal momentum appear to follow each other if between them there are only lines marked 0 or 1.

Insertion of connected clusters γ of such lines on a line l_0 of θ_1 leads to define a matrix $M^{(1)}$ formed by summing tree values of clusters γ with lines of scales 0 or 1 evaluated with the line factors defined in [107] and with the restriction that in γ there are no pairs of lines $\ell < \ell'$ with the same current and which follow each other while any line between them has lower scale (i.e., 0), here "between" means "preceding l' but not preceding l," as above.

Therefore, a scale-independent method has to be devised to check the convergence for $M^{(1)}$ and for the matrices to be introduced later to deal with even smaller propagators. This is achieved by the following extension of Siegel's theorem mentioned in the section "Quasiperiodicity and KAM stability":

Theorem 8 *Let ω_0 satisfy* [74] *and set $\omega = C\omega_0$. Consider the contribution to the sum in* [82] *from graphs θ in which*

(i) *no pairs $\ell' > \ell$ of lines which lie on the same path to the root carry the same current ν if all lines ℓ_1 between them have current $\nu(\ell_1)$ such that $|\omega \cdot \nu(\ell_1)| > 2|\omega \cdot \nu|$;*
(ii) *the node harmonics are bounded by $|\nu| \leq N$ for some N.*

Then the number of lines ℓ in θ with divisor $\omega \cdot \nu_\ell$ satisfying $2^{-n} < |\omega \cdot \nu_\ell| \leq 2^{-n+1}$ does not exceed $4Nk2^{-n/\tau}$, $n = 1, 2, \ldots$.

This implies, by the same estimates in [85], that the series defining $M^{(1)}$ converges. Again, it must be checked that there are cancellations implying that $M^{(1)}(\nu) = \varepsilon^2(\omega_0 \cdot \nu)^2 m^{(1)}(\nu)$ with $|m^{(1)}(\nu)| < D_0$ for the same $D_0 > 0$ and the same ε_0.

At this point, one deals with trees containing only lines carrying labels $0, 1, \geq 2$, and the line factors for the lines $\ell = \nu'\nu$ of scale 0 are $\nu_{\nu'} \cdot \nu_\nu / (\omega_0 \cdot \nu(\ell))^2$, those of the lines $\ell = \nu'\nu$ of scale 1 have line factors $\nu_{\nu'} \cdot (\omega_0 \cdot \nu(\ell)^2 - M^{(0)}(\nu(\ell)))^{-1} \nu_\nu$, and those of the lines $\ell = \nu'\nu$ of scale ≥ 2 have line factors

$$\nu_{\nu'} \cdot (\omega_0 \cdot \nu(\ell)^2 - M^{(1)}(\nu(\ell)))^{-1} \nu_\nu$$

Furthermore, no pair of lines of scale "1" or of scale "≥ 2" with the same momentum and with only lines of lower scale (i.e., of scale "0" in the first case or of scale "0", "1" in the second) between them can follow each other.

This procedure can be iterated until, after infinitely many steps, the problem is reduced to the evaluation of tree values in which each line carries a scale label n and there are no pairs of lines which follow each other and which have only lines of lower scale in between. Then the Siegel argument applies once more and the series so resumed is an absolutely convergent series of functions analytic in ε: hence the original series is convergent.

Although at each step there is a lower bound on the denominators, it would not be possible to avoid using Siegel's theorem. In fact, the lower bound would become worse and worse as the scale increases. In order to check

the estimates of the constants D_0, ε_0 which control the scale independence of the convergence of the various series, it is necessary to take advantage of the theorem, and of the absence (at each step) of the necessity of considering trees with pairs of consecutive lines with equal momentum and intermediate lines of higher scale.

One could also perform the analysis by bounding $h^{(k)}$ order by order with no resummations (i.e., without changing the line factors) and exhibiting the necessary cancellations. Alternatively, the paths that Kolmogorov, Arnol'd and Moser used to prove the first three (somewhat different) versions of the theorem, by successive approximations of the equations for the tori, can be followed.

The invariant tori are Lagrangian manifolds just as the unperturbed ones (cf. comments after [31]) and, in the case of the Hamiltonian [80], the generating function $\boldsymbol{A}\cdot\boldsymbol{\psi}+\Phi(\boldsymbol{A},\boldsymbol{\psi})$ can be expressed in terms of their parametric equations

$$\begin{aligned}
&\Phi(\boldsymbol{A},\boldsymbol{\psi}) = G(\boldsymbol{\psi}) + \boldsymbol{a}\cdot\boldsymbol{\psi} + \underset{\sim}{h}(\boldsymbol{\psi})\cdot(\boldsymbol{A}-\boldsymbol{\omega}-\Delta\underset{\sim}{h}(\boldsymbol{\psi}))\\
&\partial_{\boldsymbol{\psi}} G(\boldsymbol{\psi}) \stackrel{\text{def}}{=} -\Delta\underset{\sim}{h}(\boldsymbol{\psi}) + \underset{\sim}{h}(\boldsymbol{\psi})\partial_{\boldsymbol{\psi}}\Delta\underset{\sim}{h}(\boldsymbol{\psi}) - \boldsymbol{a}\\
&\boldsymbol{a} \stackrel{\text{def}}{=} \int(-\Delta\underset{\sim}{h}(\boldsymbol{\psi}) + \underset{\sim}{h}(\boldsymbol{\psi})\partial_{\boldsymbol{\psi}}\Delta\underset{\sim}{h}(\boldsymbol{\psi}))\frac{\mathrm{d}\boldsymbol{\psi}}{(2\pi)^{\ell}} \qquad [109]\\
&\quad = \int \underset{\sim}{h}(\boldsymbol{\psi})\partial_{\boldsymbol{\psi}}\Delta\underset{\sim}{h}(\boldsymbol{\psi})\frac{\mathrm{d}\boldsymbol{\psi}}{(2\pi)^{\ell}}
\end{aligned}$$

where $\Delta=(\boldsymbol{\omega}\cdot\partial_{\boldsymbol{\psi}})$ and the invariant torus corresponds to $\boldsymbol{A}'=\boldsymbol{\omega}$ in the map $\boldsymbol{\alpha}=\boldsymbol{\psi}+\partial_{\boldsymbol{A}}\Phi(\boldsymbol{A},\boldsymbol{\psi})$ and $\boldsymbol{A}'=\boldsymbol{A}+\partial_{\boldsymbol{\psi}}\Phi(\boldsymbol{A},\boldsymbol{\psi})$. In fact, by [109] the latter becomes $\boldsymbol{A}'=\boldsymbol{A}-\Delta\boldsymbol{h}$ and, from the second of [75] written for f depending only on the angles $\boldsymbol{\alpha}$, it is $\boldsymbol{A}=\boldsymbol{\omega}+\Delta\boldsymbol{h}$ when $\boldsymbol{A},\boldsymbol{\alpha}$ are on the invariant torus.

Note that if $\boldsymbol{a}$ exists it is necessarily determined by the third relation in [109] but the check that the second equation in [109] is soluble (i.e., that the RHS is an exact gradient up to a constant) is nontrivial. The canonical map generated by $\boldsymbol{A}\cdot\boldsymbol{\psi}+\boldsymbol{\Phi}(\boldsymbol{A},\boldsymbol{\psi})$ is also defined for $\boldsymbol{A}'$ close to $\boldsymbol{\omega}$ and foliates the neighborhood of the invariant torus with other tori: of course, for $\boldsymbol{A}'\neq\boldsymbol{\omega}$ the tori defined in this way are, in general, not invariant.

The reader is referred to Gallavotti *et al.* (2004) for more details.

Appendix 2: Coriolis and Lorentz Forces – Larmor Precession

Larmor precession refers to the motion of an electrically charged particle in a magnetic field H (in an inertial frame of reference). It is due to the Lorentz force which, on a unit mass with unit charge, produces an acceleration $\ddot{\varrho}=\boldsymbol{v}\wedge\boldsymbol{H}$ if the speed of light is $c=1$.

Therefore, if $\boldsymbol{H}=H\boldsymbol{k}$ is directed along the $\boldsymbol{k}$-axis, the acceleration it produces is the same that the Coriolis force would impress on a unit mass located in a reference frame which rotates with angular velocity $\omega_0\boldsymbol{k}$ around the $\boldsymbol{k}$-axis if $\boldsymbol{H}=2\omega_0\boldsymbol{k}$.

The above remarks imply that a homogeneous sphere electrically charged uniformly with a unit charge and freely pivoting about its center in a constant magnetic field H directed along the $\boldsymbol{k}$-axis undergoes the same motion as it would follow if not subject to the magnetic field but seen in a noninertial reference frame rotating at constant angular velocity ω_0 around the $\boldsymbol{k}$-axis if H and ω_0 are related by $H=2\omega_0$: in this frame, the Coriolis force is interpreted as a magnetic field.

This holds, however, only if the centrifugal force has zero moment with respect to the center: true in the spherical symmetry case only. In spherically nonsymmetric cases, the centrifugal forces have in general nonzero moment, so the equivalence between Coriolis force and the Lorentz force is only approximate.

The Larmor theorem makes this more precise. It gives a quantitative estimate of the difference between the motion of a general system of particles of mass m in a magnetic field and the motion of the same particles in a rotating frame of reference but in the absence of a magnetic field. The approximation is estimated in terms of the size of the Larmor frequency $eH/2mc$, which should be small compared to the other characteristic frequencies of the motion of the system: the physical meaning is that the centrifugal force should be small compared to the other forces.

The vector potential $\boldsymbol{A}$ for a constant magnetic field in the $\boldsymbol{k}$-direction, $\boldsymbol{H}=2\omega_0\boldsymbol{k}$, is $\boldsymbol{A}=2\omega_0\boldsymbol{k}\wedge\varrho\equiv 2\omega_0\varrho^{\perp}$. Therefore, from the treatment of the Coriolis force in the section "Three-body problem" (see [95]), the motion of a charge e with mass m in a magnetic field H with vector potential $\boldsymbol{A}$ and subject to other forces with potential W can be described, in an inertial frame and in generic units, in which the speed of light is c, by a Hamiltonian

$$\mathcal{H}=\frac{1}{2m}\left(p-\frac{e}{c}A\right)^2+W(\varrho) \qquad [110]$$

where $p=m\dot{\varrho}+(e/c)\boldsymbol{A}$ and ϱ are canonically conjugate variables.

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Introductory Article: Differential Geometry

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Differential geometry is the study of differential properties of geometric objects such as curves, surfaces and higher-dimensional manifolds endowed with additional structures such as metrics and connections. One of the main ideas of differential geometry is to apply the tools of analysis to investigate geometric problems; in particular, it studies their "infinitesimal parts," thereby linearizing the problem. However, historically, geometric concepts often anticipated the analytic tools required to define them from a differential geometric point of view; the notion of tangent to a curve, for example, arose well before the notion of derivative.

In its barely more than two centuries of existence, differential geometry has always had strong (often two-way) interactions with physics. Just to name a few examples, the theory of curves is used in kinematics, symplectic manifolds arise in Hamiltonian mechanics, pseudo-Riemannian manifolds in general relativity, spinors in quantum mechanics, Lie groups and principal bundles in gauge theory, and infinite-dimensional manifolds in the path-integral approach to quantum field theory.

Curves and Surfaces

The study of differential properties of curves and surfaces resulted from a combination of the coordinate method (or analytic geometry) developed by Descartes and Fermat during the first half of the seventeenth century and infinitesimal calculus developed by Leibniz and Newton during the second half of the seventeenth and beginning of the eighteenth century.

Differential geometry appeared later in the eighteenth century with the works of Euler *Recherches sur la courbure des surfaces* (1760) (Investigations on the curvature of surfaces) and Monge *Une application de l'analyse à la géométrie* (1795) (An application of analysis to geometry). Until Gauss' fundamental article *Disquisitiones generales circa superficies curvas* (General investigations of curved surfaces) published in Latin in 1827 (of which one can find a partial translation to English in Spivak (1979)), surfaces embedded in $\mathbb{R}^3$ were either described by an equation, $W(x, y, z) = 0$, or by expressing one variable in terms of the others. Although Euler had already noticed that the coordinates of a point on a surface could be expressed as functions of two independent variables, it was Gauss who first made a systematic use of such a parametric representation, thereby initiating the concept of "local chart" which underlies differential geometry.

Differentiable Manifolds

The actual notion of n-manifold independent of a particular embedding in a Euclidean space goes back to a lecture *Über die Hypothesen, welche der Geometrie zu Grunde liegen* (On the hypotheses which lie at the foundations of geometry) (of which one can find a translation to English and comments in Spivak (1979)) delivered by Riemann at Göttingen University in 1854, in which he makes clear the fact that n-manifolds are locally like n-dimensional Euclidean space. In his work, Riemann mentions the existence of infinite-dimensional manifolds, such as function spaces, which today play an important role since they naturally arise as configuration spaces in quantum field theories.

In modern language a differentiable manifold modeled on a topological space V (which can be

finite dimensional, Fréchet, Banach, or Hilbert for example) is a topological space M equipped with a family of local coordinate charts $(U_i, \phi_i)_{i\in I}$ such that the open subsets $U_i \subset M$ cover M and where $\phi_i : U_i \to V$, $i \in I$, are homeomorphisms which give rise to smooth transition maps $\phi_i \circ \phi_j^{-1} : \phi_j(U_i \cap U_j) \to \phi_i(U_i \cap U_j)$. An n-dimensional differentiable manifold is a differentiable manifold modeled on $\mathbb{R}^n$. The sphere $S^{n-1} := \{(x_1, \ldots, x_n) \in \mathbb{R}^n, \sum_{i=1}^n x_i^2 = 1\}$ is a differentiable manifold of dimension $n-1$.

Simple differentiable curves in $\mathbb{R}^n$ are one-dimensional differentiable manifolds locally specified by coordinates $x(t) = (x_1(t), \ldots, x_n(t)) \in \mathbb{R}^n$, where $t \mapsto x_j(t)$ is of class C^k. The tangent at point $x(t_0)$ to such a curve, which is a straight line passing through this point with direction given by the vector $x'(t_0)$, generalizes to the concept of tangent space T_mM at point $m \in M$ of a smooth manifold M modeled on V which is a vector space isomorphic to V spanned by tangent vectors at point m to curves $\gamma(t)$ of class C^1 on M such that $\gamma(t_0) = m$.

In order to make this more precise, one needs the notion of differentiable mapping. Given two differentiable manifolds M and N, a mapping $f : M \to N$ is differentiable at point m if, for every chart (U, ϕ) of M containing m and every chart (V, ψ) of N such that $f(U) \subset V$, the mapping $\psi \circ f \circ \phi^{-1} : \phi(U) \to \psi(V)$ is differentiable at point $\phi(m)$. In particular, differentiable mappings $f : M \to \mathbb{R}$ form the algebra $C^\infty(M, \mathbb{R})$ of smooth real-valued functions on M. Differentiable mappings $\gamma : [a, b] \to M$ from an interval $[a, b] \subset \mathbb{R}$ to a differentiable manifold M are called "differentiable curves" on M. A differentiable mapping $f : M \to N$ which is invertible and with differentiable inverse $f^{-1} : N \to M$ is called a diffeomorphism.

The derivative of a function $f \in C^\infty(M, \mathbb{R})$ along a curve $\gamma : [a, b] \to M$ at point $\gamma(t_0) \in M$ with $t_0 \in [a, b]$ is given by

$$Xf := \frac{\mathrm{d}}{\mathrm{d}t}_{|_{t=t_0}} f \circ \gamma(t)$$

and the map $f \mapsto Xf$ is called the tangent vector to the curve γ at point $\gamma(t_0)$. Tangent vectors to some curve $\gamma : [a, b] \to M$ at a given point $m \in \gamma([a, b])$ form a vector space T_mM called the "tangent space" to M at point m.

A (smooth) map which, to a point $m \in M$, assigns a tangent vector $X \in T_mM$ is called a (smooth) vector field. It can also be seen as a derivation $\tilde{X} : f \mapsto Xf$ on $C^\infty(M, \mathbb{R})$ defined by $(\tilde{X}f)(m) := X(m)f$ for any $m \in M$ and the bracket of vector fields is thereby defined from the operator bracket $[\widetilde{X, Y}] := \tilde{X} \circ \tilde{Y} - \tilde{Y} \circ \tilde{X}$. The linear operations on tangent vectors carry out to vector fields $(X + Y)(m) := X(m) + Y(m)$, $(\lambda X)(m) := \lambda X(m)$ for any $m \in M$ and for any $X, Y \in T_mM, \lambda \in \mathbb{R}$ so that vector fields on M build a linear space.

One can generate tangent vectors to M via local one-parameter groups of differentiable transformations of M, that is, mappings $(t, m) \mapsto \phi_t(m)$ from $]-\epsilon, \epsilon[\times U$ to U (with $\epsilon > 0$ and $U \subset M$ an open subset of M) such that $\phi_0 = \mathrm{Id}$, $\phi_{t+s} = \phi_t \circ \phi_s$ $\forall s, t \in]-\epsilon, \epsilon[$ with $t + s \in]-\epsilon, \epsilon[$ and $m \mapsto \phi_t(m)$ is a diffeomorphism of U onto an open subset $\phi_t(U)$. The tangent vector at $t = 0$ to the curve $\gamma(t) = \phi_t(m)$ yields a tangent vector to M at point $m = \gamma(0)$. Conversely, when M is finite dimensional, the fundamental theorem for systems of ordinary equations yields, for any vector field X on M, the existence (around any point $m \in M$) of a local one-parameter group of local transformations $\phi :]-\epsilon, \epsilon[\times U \to M$ (with U an open subset containing m) which induces the tangent vector $X(m) \in T_mM$.

A differentiable mapping $\phi : M \to N$ induces a map $\phi_*(m) : T_mM \to T_{\phi(m)}M$ defined by $\phi_* Xf = X(f \circ \phi)$. An "immersion" of a manifold M in a manifold N is a differentiable mapping $\phi : M \to N$ such that the maps $\phi_*(m)$ are injective at any point $m \in M$. Such a map is an embedding if it is moreover injective in which case $\phi(M) \subset N$ is a submanifold of N. The unit sphere S^n is a submanifold of $\mathbb{R}^{n+1}$. Whitney showed that every smooth real n-dimensional manifold can be embedded in $\mathbb{R}^{2n+1}$.

A differentiable manifold whose coordinate charts take values in a complex vector space V and whose transition maps are holomorphic is called a complex manifold, which is complex n-dimensional if $V = \mathbb{C}^n$. The complex projective space $\mathbb{C}P^n$, the union of complex straight lines through 0 in $\mathbb{C}^{n+1}$, is a compact complex manifold of dimension n. Similarly to the notion of differentiable mapping between differentiable manifolds, we have the notion of holomorphic mapping between complex manifolds.

A smooth family $m \mapsto J_m$ of endomorphisms of the tangent spaces T_mM to a differentiable manifold M such that $J_m^2 = -\mathrm{Id}$ gives rise to an almost-complex manifold. The prototype is the almost-complex structure on $\mathbb{C}^n$ defined by $J(\partial_{x_i}) = \partial_{y_i}$; $J(\partial_{y_i}) = -\partial_{x_i}$ with $z = (x_1 + \mathrm{i}y_1, \ldots, x_n + \mathrm{i}y_n) \in \mathbb{C}^n$ which can be transferred to a complex manifold M by means of local charts. An almost-complex structure J on a manifold M is called complex if M is the underlying differentiable manifold of a complex manifold which induces J in this way.

Studying smooth functions on a differentiable manifold can provide information on the topology of the manifold: for example, the behavior of a smooth function on a compact manifold as its critical points strongly restricted by the topological properties of the manifold. This leads to the Morse

critical point theory which extends to infinite-dimensional manifolds and, among other consequences, leads to conclusions on extremals or closed extremals of variational problems. Rather than privileging points on a manifold, one can study instead the geometry of manifolds from the point of view of spaces of functions, which leads to an algebraic approach to differential geometry. The initial concept there is a commutative ring (which becomes a possibly noncommutative algebra in the framework of noncommutative geometry), namely the ring of smooth functions on the manifold, while the manifold itself is defined in terms of the ring as the space of maximal ideals. In particular, this point of view proves to be fruitful to understand supermanifolds, a generalization of manifolds which is important for supersymmetric field theories.

One can further consider the sheaf of smooth functions on an open subset of the manifold; this point of view leads to sheaf theory which provides a unified approach to establishing connections between local and global properties of topological spaces.

Metric Properties

Riemann focused on the metric properties of manifolds but the first clear formulation of the concept of a manifold equipped with a metric was given by Weyl in *Die Idee der Riemannsche Fläche*. A Riemannian metric on a differentiable manifold M is a positive-definite scalar product g_m on T_mM for every point $m \in M$ depending smoothly on the point m. A manifold equipped with a Riemannian metric is called a Riemannian manifold. A Weyl transformation, which is multiplying the metric by a smooth positive function, yields a new Riemannian metric with the same angle measurement as the original one, and hence leaves the "conformal" structure on M unchanged.

Riemann also suggested considering metrics on the tangent spaces that are not induced from scalar products; metrics on the manifold built this way were first systematically investigated by Finsler and are therefore called Finsler metrics. Geodesics on a Riemannian manifold M which correspond to smooth curves $\gamma : [a, b] \to M$ that minimize the length functional

$$L(\gamma) := \frac{1}{2}\int_a^b \sqrt{g_{\gamma(t)}\left(\frac{\mathrm{d}\gamma}{\mathrm{d}t}, \frac{\mathrm{d}\gamma}{\mathrm{d}t}\right)}\,\mathrm{d}t$$

then generalize to curves which realize the shortest distance between two points chosen sufficiently close.

Euclid's axioms which naturally lead to Riemannian geometry are also satisfied up to the axiom of parallelism by a geometry developed by Lobatchevsky in 1829 and Bolyai in 1832. Non-Euclidean geometries actually played a major role in the development of differential geometry and Lobachevsky's work inspired Riemann and later Klein.

Dropping the positivity assumption for the bilinear forms g_m on T_mM leads to Lorentzian manifolds which are $(n+1)$-dimensional smooth manifolds equipped with bilinear forms on the tangent spaces with signature $(1, n)$. These occur in general relativity and tangent vectors with negative, positive, or vanishing squared length are called timelike, spacelike, and lightlike, respectively.

Just as complex vector spaces can be equipped with positive-definite Hermitian products, a complex manifold M can come equipped with a Hermitian metric, namely a positive-definite Hermitian product h_m on T_mM for every point $m \in M$ depending smoothly on the point m; every Hermitian metric induces a Riemannian one given by its real part. The complex projective space CP^n comes naturally equipped with the Fubini–Study Hermitian metric.

Transformation Groups

Metric properties can be seen from the point of view of transformation groups. Poncelet in his *Traité projectif des figures* (1822) had investigated classical Euclidean geometry from a projective geometric point of view, but it was not until Cayley (1858) that metric properties were interpreted as those stable under any "projective" transformation which leaves "cyclic points" (points at infinity on the imaginary axis of the complex plane) invariant. Transformation groups were further investigated by Lie, leading to the modern concept of Lie group, a smooth manifold endowed with a group structure such that the group operations are smooth.

A vector field X on a Lie group G is called left- (resp. right-) invariant if it is invariant under left translations $L_g : h \mapsto gh$ (resp. right translations $R_g : h \mapsto hg$) for every $g \in G$, that is, if $(L_g)_* X(h) = X(gh)\ \forall (g, h) \in G^2$ (resp. $(R_g)_* X(h) = X(gh)\ \forall (g, h) \in G^2$). The set of all left-invariant vector fields equipped with the sum, scalar multiplication, and the bracket operation on vector fields form an algebra called the Lie algebra of G.

The group $\mathrm{Gl}_n(\mathbb{R})$ (resp. $\mathrm{Gl}_n(\mathbb{C})$) of all real (resp. complex) invertible $n \times n$ matrices is a Lie group with Lie algebra, the algebra $\mathrm{gl}_n(\mathbb{R})$ (resp. $\mathrm{gl}_n(\mathbb{C})$) of all real (resp. complex) $n \times n$ matrices and the bracket operation reads $[A, B] = AB - BA$.

The orthogonal (resp. unitary) group $\mathrm{O}_n(\mathbb{R}) := \{A \in \mathrm{Gl}_n(\mathbb{R}), A^{\mathrm{t}}A = 1\}$, where A^{t} denotes the transposed matrix (resp. $U_n(\mathbb{C}) := \{A \in \mathrm{Gl}_n(\mathbb{C}),\ A^*A = 1\}$, where $A^* = \bar{A}^{\mathrm{t}}$), is a compact Lie group with Lie

algebra $o_n(\mathbb{R}) := \{A \in \mathrm{Gl}_n(\mathbb{R}), A^t = -A\}$ (resp. $u_n(\mathbb{C}) := \{A \in \mathrm{Gl}_n(\mathbb{C}), A^* = -A\}$).

A left-invariant vector field X on a finite-dimensional Lie group G (or equivalently an element X of the Lie algebra of G) generates a global one-parameter group of transformations $\phi_X(t), t \in \mathbb{R}$. The mapping from the Lie algebra of G into G defined by $\exp(X) := \phi_X(1)$ is called the exponential mapping. The exponential mapping on $\mathrm{Gl}_n(\mathbb{R})$ (resp. $\mathrm{Gl}_n(\mathbb{C})$) is given by the series $\exp(A) = \sum_{i=0}^{\infty} A^i/i!$.

As symmetry groups of physical systems, Lie groups play an important role in physics, in particular in quantum mechanics and Yang–Mills theory. Infinite-dimensional Lie groups arise as symmetry groups, such as the group of diffeomorphisms of a manifold in general relativity, the group of gauge transformations in Yang–Mills theory, and the group of Weyl transformations of metrics on a surface in string theory. The principle "the physics should not depend on how it is described" translates to an invariance under the action of the (possibly infinite-dimensional group) of symmetries of the theory. Anomalies arise when such an invariance holds for the classical action of a physical theory but "breaks" at the quantized level.

In his Erlangen program (1872), Klein puts the concept of transformation group in the foreground introducing a novel idea by which one should consider a space endowed with some properties as a set of objects invariant under a given group of transformations. One thereby reaches a classification of geometric results according to which group is relevent in a particular problem as, for example, the projective linear group for projective geometry, the orthogonal group for Riemannian geometry, or the symplectic group for "symplectic" geometry.

Fiber Bundles

Transformation groups give rise to principal fiber bundles which play a major role in Yang–Mills theory. The notion of fiber bundle first arose out of questions posed in the 1930s on the topology and the geometry of manifolds, and by 1950 the definition of fiber bundle had been clearly formulated by Steenrod.

A smooth fiber bundle with typical fiber a manifold F is a triple (E, π, B), where E and B are smooth manifolds called the total space and the base space, and $\pi : E \to B$ is a smooth surjective map called the projection of the bundle such that the preimage $\pi^{-1}(b)$ of a point $b \in B$ called the fiber of the bundle over b is isomorphic to F and any base point b has a neighborhood $U \subset B$ with preimage $\pi^{-1}(U)$ diffeomorphic to $U \times F$, where the diffeomophisms commute with the projection on the base space. Smooth sections of E are maps $\sigma : B \to E$ such that $\pi \circ \sigma = I_B$.

When F is a vector space and when, given open subsets $U_i \subset B$ that cover B with corresponding coordinate charts $(U_i, \phi_i)_{i \in I}$, the local diffeomorphisms $\tau_i : \pi^{-1}(U_i) \simeq \phi_i(U_i) \times F$ give rise to transition maps $\tau_i \circ \tau_j^{-1} : \phi_j(U_i \cap U_j) \times F \to \phi_i(U_i \cap U_j) \times F$ that are linear in the fiber, the bundle is called a "vector bundle." The tangent bundle $TM = \bigcup_{m \in M} T_m M$ to a differentiable manifold M modeled on a vector space V is a vector bundle with typical fiber V and transition maps $\tau_{ij} = (\phi_i \circ \phi_j^{-1}, \mathrm{d}(\phi_i \circ \phi_j^{-1}))$ expressed in terms of the differentials of the transition maps on the manifold M. So are the cotangent bundle, the dual of the tangent bundle, and tensor products of the tangent and cotangent vector bundles with typical fiber the dual V^* and tensor products of V and V^*. Vector fields defined previously are sections of the tangent bundle, 1-forms on M are sections of the cotangent bundle, and contravariant tensors, resp. covariant tensors are sections of tensor products of the tangent, resp. cotangent bundles. A differentiable mapping $\phi : M \to N$ takes covariant p-tensor fields on N to their pullbacks by ϕ, covariant p-tensors on M given by

$$(\phi^* T)(X_1, \ldots, X_p) := T(\phi_* X_1, \ldots, \phi_* X_p)$$

for any vector fields $X_1, \ldots, X_p$ on M.

Differentiating a smooth function f on M gives rise to a 1-form $\mathrm{d}f$ on M. More generally, exterior p-forms are antisymmetric smooth covariant p-tensors so that $\omega(X_{\sigma(1)}, \ldots, X_{\sigma(p)}) = \epsilon(\sigma)\omega(X_1, \ldots, X_p)$ for any vector fields $X_1, \ldots, X_p$ on M and any permutation $\sigma \in \Sigma_p$ with signature $\epsilon(\sigma)$.

Riemannian metrics are covariant 2-tensors and the space of Riemannian metrics on a manifold M is an infinite-dimensional manifold which arises as a configuration space in string theory and general relativity.

A principal bundle is a fiber bundle (P, π, B) with typical fiber a Lie group G acting freely and properly on the total space P via a right action $(p, g) \in P \times G \mapsto pg = R_g(p) \in P$ and such that the local diffeomorphisms $\pi^{-1}(U) \simeq U \times G$ are G-equivariant. Given a principal fiber bundle (P, π, B) with structure group a finite-dimensional Lie group G, the action of G on P induces a homomorphism which to an element X of the Lie algebra of G assigns a vector field X^* on P called the "fundamental vector field" generated by X. It is defined at $p \in P$ by

$$X^*(p) := \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} R_{\exp(tX)}(p)$$

where exp is the exponential map on G.

Given an action of G on a vector space V, one builds from a principal bundle with typical fiber G an associated vector bundle with typical fiber V. Principal bundles are essential in gauge theory; $U(1)$-principal bundles arise in electro-magnetism and nonabelian structure groups arise in Yang–Mills theory. There the fields are connections on the principal bundle, and the action of gauge transformations on (irreducible) connections gives rise to an infinite-dimensional principal bundle over the moduli space with structure group given by gauge transformations. Infinite-dimensional bundles arise in other field theories such as string theory where the moduli space corresponds to inequivalent complex structures on a Riemann surface and the infinite-dimensional structure group is built up from Weyl transformations of the metric and diffeomorphisms of the surface.

Connections

On a manifold there is no canonical method to identify tangent spaces at different points. Such an identification, which is needed in order to differentiate vector fields, can be achieved on a Riemannian manifold via "parallel transport" of the vector fields. The basic concepts of the theory of covariant differentiation on a Riemannian manifold were given at the end of the nineteenth century by Ricci and, in a more complete form, in 1901 in collaboration with Levi-Civita in *Méthodes de calcul différentiel absolu et leurs applications*; on a Riemannian manifold, it is possible to define in a canonical manner a parallel displacement of tangent vectors and thereby to differentiate vector field covariantly using the since then called Levi-Civita connection.

More generally, a (linear) connection (or equivalently a covariant derivation) on a vector bundle E over a manifold M provides a way to identify fibers of the vector bundle at different points; it is a map ∇ taking sections σ of E to E-valued 1-forms on M which satisfies a Leibniz rule, $\nabla(f\sigma) = \mathrm{d}f\sigma + f\nabla\sigma$, for any smooth function f on M. When E is the tangent bundle over M, curves γ on the manifold with covariantly constant velocity $\nabla\dot{\gamma}(t) = 0$ give rise to geodesics. Given an initial velocity $\dot{\gamma}(0) = X \in T_mM$ and provided X has small enough norm, $\gamma_X(1)$ defines a point on the corresponding geodesic and the map $exp : X \mapsto \gamma_X(1)$ a diffeomorphism from a neighborhood of 0 in T_mM to a neighborhood of $m \in M$ called the "exponential map" of ∇.

The concept of connection extends to principal bundles where it was developed by Ehresmann building on the work of Cartan. A connection on a principal bundle (P, π, B) with structure group G, which is a smooth equivariant (under the action of the group G) decomposition of the tangent space $T_pP = H_pP \oplus V_pP$ at each point p into a horizontal space H_pP and the vertical space $V_pP = \mathrm{Ker}\,\mathrm{d}\pi_p$, gives rise to a linear connection on the associated vector bundle.

A connection on P gives rise to a 1-form ω on P with values in the Lie algebra of the structure group G called the connection 1-form and defined as follows. For each $X \in T_pP, \omega(X)$ is the unique element U of the Lie algebra of G such that the corresponding fundamental vector field $U^*(p)$ at point p coincides with the vertical component of X. In particular, $\omega(U^*) = U$ for any element U of the Lie algebra of G.

The space of connections which is an infinite-dimensional manifold arises as a configuration space in Yang–Mills theory and also comes into play in the Seiberg–Witten theory.

Geometric Differential Operators

From connections one defines a number of differential operators on a Riemannian manifold, among them second-order Laplacians. In particular, the Laplace–Beltrami operator $f \mapsto -\mathrm{tr}(\nabla^{T^*M}\mathrm{d}f)$ on smooth functions, where ∇^{T^*M} is the connection on the cotangent bundle induced by the Levi-Civita connection on M, generalizes the ordinary Laplace operator on Euclidean space. This in turn generalizes to second-order operators $\Delta^E := -\mathrm{tr}(\nabla^{T^*M\otimes E}\nabla^E)$ acting on smooth sections of a vector bundle E over a Riemannian manifold M, where ∇^E is a connection on E and $\nabla^{T^*M\otimes E}$ the connection on $T^*M \otimes E$ induced by ∇^E and the Levi-Civita connection on M.

The Dirac operator on a spin Riemannian manifold, a first-order differential operator whose square coincides with the Laplace–Beltrami operator up to zeroth-order terms, can be best understood going back to the initial idea of Dirac. A first-order differential operator with constant matrix coefficients $\sum_{i=1}^n \gamma_i(\partial/\partial x_i)$ has square given by the Laplace operator $-\sum_{i=1}^n \partial^2/\partial x_i^2$ on $\mathbb{R}^n$ if and only if its coefficients satisfy the the Clifford relations

$$\gamma_i^2 = -1 \quad \forall\, i = 1, \ldots, n$$
$$\gamma_i\gamma_j + \gamma_j\gamma_i = 0 \quad \forall\, i \neq j$$

The resulting Clifford algebra, once complexified, is isomorphic in even dimensions $n = 2k$ to the space $\mathrm{End}(S_n)$ (and $\mathrm{End}(S_n) \oplus \mathrm{End}(S_n)$ in odd dimensions $n = 2k + 1$) of endomorphisms of the space $S_n = \mathbb{C}^{2^k}$ of complex n-spinors. When instead of the canonical metric on $\mathbb{R}^n$ one starts from the the metric on the tangent bundle TM induced by the Riemannian

metric on M and provided the corresponding spinor spaces patch up to a "spinor bundle" over M, M is called a spin manifold. The Dirac operator on a spin Riemannian manifold M is a first-order differential operator acting on spinors given by $D_g = \sum_{i=1}^{n} \gamma_i \nabla_{e_i}$, where ∇ is the connection on spinors (sections of the spinor bundle S) induced by the Levi-Civita connection and $e_1, \ldots, e_n$ is an orthonormal frame of the tangent bundle TM. This is a particular case of more general twisted Dirac operators D_g^W on a twisted spinor bundle $S \otimes W$ equipped with the connection $\nabla^{S\otimes W}$ which combines the connection ∇ with a connection ∇^W on an auxilliary vector bundle W. Their square $(D_g^W)^2$ relates to the Laplacian $\Delta^{S\otimes W}$ built from this twisted connection via the Lichnerowicz formula which is useful for estimates on the spectrum of the Dirac operator in terms of the underling geometric data.

When there is no spin structure on M, one can still hope for a Spin^c structure and a Dirac D^c operator associated with a connection compatible with that structure. In particular, every compact orientable 4-manifold can be equipped with a Spin^c structure and one can build invariants of the differentiable manifold called Seiberg–Witten invariants from solutions of a system of two partial differential equations, one of which is the Dirac equation $D^c\Phi = 0$ associated with a connection compatible with the Spin^c structure and the other a nonlinear equation involving the curvature.

Curvature

The concept of "curvature," which is now understood in terms of connections (the curvature of a connection ∇ is defined by $\Omega = \nabla^2$), historically arose prior to that of connection. In its modern form, the concept of curvature dates back to Gauss. Using a spherical representation of surfaces – the Gauss map ν, which sends a point m of an oriented surface $\Sigma \subset \mathbb{R}^3$ to the outward pointing unit normal vector ν_m – Gauss defined what is since then called the Gaussian curvature K_m at point $m \in U \subset \Sigma$ as the limit when the area of U tends to zero of the ratio $\text{area}(\nu(U))/\text{area}(U)$. It measures the obstruction to finding a distance-preserving map from a piece of the surface around m to a region in the standard plane. Gauss' *Teorema Egregium* says that the Gaussian curvature of a smooth surface in $\mathbb{R}^3$ is defined in terms of the metric on the surface so that it agrees for two isometric surfaces.

From the curvature Ω of a connection on a Riemannian manifold (M, g), one builds the Riemannian curvature tensor, a 4-tensor which in local coordinates reads

$$R_{ijkl} := g\left(\Omega\left(\frac{\partial}{\partial_i}, \frac{\partial}{\partial_j}\right)\frac{\partial}{\partial_k}, \frac{\partial}{\partial_l}\right)$$

further taking a partial trace leads to the Ricci curvature given by the 2-tensor $\text{Ric}_{ij} = \sum_k R_{ikjk}$, the trace of which gives in turn the scalar curvature $R = \sum_i \text{Ric}_{ii}$. Sectional curvature at a point m in the direction of a two-dimensional plane spanned by two vectors U and V corresponds to $K(U, V) = g(\Omega(U, V)V, U)$. A manifold has constant sectional curvature whenever $K(U, V)/\|U \wedge V\|^2$ is a constant K for all linearly independent vectors U, V. A Riemannian manifold with constant sectional curvature is said to be spherical, flat, or hyperbolic type depending on whether $K > 0, K = 0$, or $K < 0$, respectively. One owes to Cartan the discovery of an important class of Riemannian manifolds, symmetric spaces, which contains the spheres, the Euclidean spaces, the hyperbolic spaces, and compact Lie groups. A connected Riemannian manifold M equipped at every point m with an isometry σ_m such that $\sigma_m(m) = m$ and the tangent map $T_m\sigma_m$ equals –Id on the tangent space (it therefore reverses the geodesics through m) is called symmetric. $\mathbb{C}P^n$ equipped with the Fubini–Study metric is a symmetric space with the isometry given by the reflection with respect to a line in $\mathbb{C}^{n+1}$. A compact symmetric space has non-negative sectional curvature K.

Constraints on the curvature can have topological consequences. Spheres are the only simply connected manifolds with constant positive sectional curvature; if a simply connected complete Riemannian manifold of dimension >1 has non-positive sectional curvature along every plane, then it is homeomorphic to the Euclidean space.

A manifold with Ricci curvature tensor proportional to the metric tensor is called an Einstein manifold. Since Einstein, curvature is a cornerstone of general relativity with gravitational force being interpreted in terms of curvature. For example, the vacuum Einstein equation reads $\text{Ric}_g = (1/2)R_g\, g$ with Ric_g the Ricci curvature of a metric g and R_g its scalar curvature. In addition, Kaluza–Klein supergravity is a unified theory modeled on a direct product of the Mikowski four-dimensional space and an Einstein manifold with positive scalar curvature.

The Ricci flow $dg(t)/dt = -2\text{Ric}_{g(t)}$, which is related with the Einstein equation in general relativity, was only fairly recently introduced in the mathematical literature. Hopes are strong to get a classification of closed 3-manifolds using the Ricci flow as an essential ingredient.

Cohomology

Differentiation of functions $f \mapsto \mathrm{d}f$ on a differentiable manifold M generalizes to exterior differentiation $\alpha \mapsto d\alpha$ of differential forms. A form α is closed whenever it is in the kernel of d and it is exact whenever it lies in the range of d. Since $d^2 = 0$, exact forms are closed.

Cartan's structure equations $d\omega = -(1/2)[\omega, \omega] + \Omega$ relate the exterior differential of the connection 1-form ω on a principal bundle to its curvature Ω given by the exterior covariant derivative $D\omega := d\omega \circ h$, where $h : T_pP \to H_pP$ is the projection onto the horizontal space.

On a complex manifold, forms split into sums of (p, q)-forms, those with p-holomorphic and q-antiholomorphic components, and exterior differentiation splits as $d = \partial + \bar{\partial}$ into holomorphic and antiholomorphic derivatives, with $\partial^2 = \bar{\partial}^2 = 0$.

Geometric data are often expressed in terms of closedness conditions on certain differential forms. For example, a "symplectic manifold" is a manifold M equipped with a closed nondegenerate differential 2-form called the "symplectic form." The theory of J-holomorphic curves on a manifold equipped with an almost-complex structure J has proved fruitful in building invariants on symplectic manifolds. A Kähler manifold is a complex manifold equipped with a Hermitian metric h whose imaginary part $\mathrm{Im}\, h$ yields a closed $(1, 1)$-form. The complex projective space $\mathbb{C}P^n$ is Kähler.

The exterior differentation d gives rise to de Rham cohomology as $\mathrm{Ker}\, d/\mathrm{Im}\, d$, and de Rham's theorem establishes an isomorphism between de Rham cohomology and the real singular cohomology of a manifold. Chern (or characteristic) classes are topological invariants associated to fiber bundles and play a crucial role in index theory. Chern–Weil theory builds representatives of these de Rham cohomology classes from a connection ∇ of the form $\mathrm{tr}(f(\nabla^2))$, where f is some analytic function.

When the manifold is Riemannian, the Laplace–Beltrami operator on functions generalizes to differential forms in two different ways, namely to the Bochner Laplacian $\Delta^{\Lambda T^*M}$ on forms (i.e., sections of ΛT^*M), where the contangent bundle T^*M is equipped with a connection induced by the Levi-Civita connection and to the Laplace–Beltrami operator on forms $(d + d^*)^2 = d^*d + d\,d^*$, where d^* is the (formal) adjoint of the exterior differential d. These are related via Weitzenböck's formula which in the particular case of 1-forms states that the difference of those two operators is measured by the Ricci curvature.

When the manifold is compact, Hodge's theorem asserts that the de Rham cohomology groups are isomorphic to the space of harmonic (i.e., annihilated by the Laplace–Beltrami operator) differential forms. Thus, the dimension of the set of harmonic k-forms equals the kth Betti numbers from which one can define the Euler characteristic $\chi(M)$ of the manifold M taking their alternate sum. Hodge theory plays an important role in mirror symmetry which posits a duality between different manifolds on the geometric side and between different field theories via their correlation functions on the physics side. Calabi–Yau manifolds, which are Ricci-flat Kähler manifolds, are studied extensively in the context of duality.

Index Theory

While the Gaussian curvature is the solution to a local problem, it has strong influence on the global topology of a surface. The Gauss–Bonnet formula (1850) relates the Euler characteristic on a closed surface to the Gaussian curvature by

$$\chi(M) = \frac{1}{2\pi} \int_M K_m \, \mathrm{d}A_m$$

where $\mathrm{d}A_m$ is the volume element on M. This is the first result relating curvature to global properties and can be seen as one of the starting points for index theory. It generalizes to the Chern–Gauss–Bonnet theorem (1944) on an even-dimensional closed manifold and can be interpreted as an example of the Atiyah–Singer index theorem (1963)

$$\mathrm{ind}(D_g^W) = \int_M \hat{A}(\Omega_g)\, \mathrm{e}^{-\mathrm{tr}(\Omega^W)}$$

where g denotes a Riemannian metric on a spin manifold M, D_g^W a Dirac operator acting on sections of some twisted bundle $S \otimes W$ with S the spinor bundle on M and W an auxiliary vector bundle over M, $\mathrm{ind}(D_g^W)$ the "index" of the Dirac operator, and Ω_g, Ω^W respectively the curvatures of the Levi-Civita connection and a connection on W, and $\hat{A}(\Omega_g)$ a particular Chern form called the $\hat{A}$-genus. Index theorems are useful to compute anomalies in gauge theories arising from functional quantisation of classical actions.

Given an even-dimensional closed spin manifold (M, g) and a Hermitian vector bundle W over M, the index of the associated Dirac operator D_g^W yields the so-called Atiyah map $K^0(M) \mapsto \mathbb{Z}$ defined by $W \mapsto \mathrm{ind}(D_g^W)$, where $K^0(M)$ is the group of formal differences of stable homotopy classes of smooth vector bundles over M. This is the starting point for the noncommutative geometry approach to index theory, in which the space of smooth functions on a

manifold which arises here in a disguised from since $K^0(M) \simeq K_0(C^\infty(M))$ (which consists of formal differences of smooth homotopy classes of idempotents in the inductive limit of spaces of matrices $gl_n(C^\infty(M))$) is generalized to any noncommutative smooth algebra.

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Introductory Article: Electromagnetism

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Introduction

The modern theory of electromagnetism is built on the foundations of Maxwell's equations:

$$\operatorname{div} \boldsymbol{E} = \frac{\rho}{\epsilon_0} \quad [1]$$

$$\operatorname{div} \boldsymbol{B} = 0 \quad [2]$$

$$\operatorname{curl} \boldsymbol{B} - \frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} = \mu_0 \boldsymbol{J} \quad [3]$$

$$\operatorname{curl} \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0 \quad [4]$$

On the left-hand side are the electric and magnetic fields, $\boldsymbol{E}$ and $\boldsymbol{B}$, which are vector-valued functions of position and time. On the right are the sources, the charge density ρ, which is a scalar function of position and time, and the current density $\boldsymbol{J}$. The source terms encode the distribution and velocities of charges, and the equations, together with boundary conditions at infinity, determine the fields that they generate. From these equations, one can derive the familiar predictions of electrostatics and magnetostatics, as well as the dynamical behavior of fields and charges, in particular, the generation and propagation of electromagnetic waves – light waves.

Maxwell would not have recognized the equations in this compact vector notation – still less in the tensorial form that they take in special relativity. It is notable that although his contribution is universally acknowledged in the naming of the equations, it is rare to see references to "Maxwell's theory." This is for a good reason. In his early studies of electromagnetism, Maxwell worked with elaborate mechanical models, which he saw as analogies rather than as literal descriptions of the underlying physical reality. In his later work, the mechanical models, in particular the mechanical properties of the "lumiferous ether" through which light waves propagate, were put forward more literally as the foundations of his electromagnetic theory. The equations survive in the modern theory, but the mechanical models with which Maxwell, Faraday, and others wrestled live on only in the survival of archaic terminology, such as "lines of force" and "magnetic flux." The luminiferous ether evaporated with the advent of special relativity.

Maxwell's legacy is not his "theory," but his equations: a consistent system of partial differential equations that describe the whole range of known interactions of electric and magnetic fields with

moving charges. They unify the treatment of electricity and magnetism by revealing for the first time the full duality between the electric and magnetic fields. They have been verified over an almost unimaginable variety of physical processes, from the propagation of light over cosmological distances, through the behavior of the magnetic fields of stars and the everyday applications in electrical engineering and laboratory experiments, down – in their quantum version – to the exchange of photons between individual electrons.

The history of Maxwell's equations is convoluted, with many false turns. Maxwell himself wrote down an inconsistent form of the equations, with a different sign for ρ in the first equation, in his 1865 work "A dynamical theory of the electromagnetic field." The consistent form appeared later in his *Treatise on Electricity and Magnetism* (1873); see Chalmers (1975).

In this article, we shall not follow the historical route to the equations. Some of the complex story of the development hinted at in the remarks above can be found in the articles by Chalmers (1975), Siegel (1985), and Roche (1998). Neither shall we follow the traditional pedagogic route of many textbooks in building up to the full dynamical equations through the study of basic electrical and magnetic phenomena. Instead, we shall follow a path to Maxwell's equations that is informed by knowledge of their most critical feature, invariance under Lorentz transformations. Maxwell, of course, knew nothing of this.

We shall start with a summary of basic facts about the behavior of charges in electric and magnetic fields, and then establish the full dynamical framework by considering this behavior as seen from moving frames of reference. It is impossible, of course, to do this consistently within the framework of classical ideas of space and time since Maxwell's equations are inconsistent with Galilean relativity. But it is at least possible to understand some of the key features of the equations, in particular the need for the term involving the time derivative of E, the so-called "displacement current," in the third of Maxwell's equations.

We shall begin with some remarks concerning the role of relativity in classical dynamics.

Relativity in Newtonian Dynamics

Newton's laws hold in all inertial frames. The formalism of classical mechanics is invariant under Galilean transformations and it is impossible to tell by observing the dynamical behavior of particles and other bodies whether a frame of reference is at rest or in uniform motion. In the world of classical mechanics, therefore:

Principle of Relativity There is no absolute standard of rest; only relative motion is observable.

In his "Dialogue concerning the two chief world systems," Galileo illustrated the principle by arguing that the uniform motion of a ship on a calm sea does not affect the behavior of fish, butterflies, and other moving objects, as observed in a cabin below deck.

Relativity theory takes the principle as fundamental, as a statement about the nature of space and time as much as about the properties of the Newtonian equations of motion. But if it is to be given such universal significance, then it must apply to all of physics, and not just to Newtonian dynamics. At first this seems unproblematic – it is hard to imagine that it holds at such a basic level, but not for more complex physical interactions. Nonetheless, deep problems emerge when we try to extend it to electromagnetism since Galilean invariance conflicts with Maxwell's equations.

All appears straightforward for systems involving slow-moving charges and slowly varying electric and magnetic fields. These are governed by laws that appear to be invariant under transformations between uniformly moving frames of reference. One can imagine a modern version of Galileo's ship also carrying some magnets, batteries, semiconductors, and other electrical components. Salviati's argument for relativity would seem just as compelling.

The problem arises when we include rapidly varying fields – in particular, when we consider the propagation of light. As Einstein (1905) put it, "Maxwell's electrodynamics..., when applied to moving bodies, leads to asymmetries which do not appear to be inherent in the phenomena." The central difficulty is that Maxwell's equations give light, along with other electromagnetic waves, a definite velocity: in empty space, it travels with the same speed in every direction, independently of the motion of the source – a fact that is incompatible with Galilean invariance. Light traveling with speed c in one frame should have speed $c+u$ in a frame moving towards the source of the light with speed u. Thus, it should be possible for light to travel with any speed. Light that travels with speed c in a frame in which its source is at rest should have some other speed in a moving frame; so Galilean invariance would imply dependence of the velocity of light on the motion of the source.

A full resolution of the conflict can only be achieved within the special theory of relativity: here, remarkably, Maxwell's equations retain exactly

their classical form, but the transformations between the space and time coordinates of frames of reference in relative motion do not. The difference appears when the velocities involved are not insignificant when compared with the velocity of light. So long as one can ignore terms of order u^2/c^2, Maxwell's equations are compatible with the Galilean principle of relativity.

Charges, Fields, and the Lorentz-Force Law

The basic objects in the modern form of electromagnetic theory are

- charged particles; and
- the electric and magnetic fields E and B, which are vector quantities that depend on position and time.

The charge e of a particle, which can be positive or negative, is an intrinsic quantity analogous to gravitational mass. It determines the strength of the particle's interaction with the electric and magnetic fields – as its mass determines the strength of its interaction with gravitational fields.

The interaction is in two directions. First, electric and magnetic fields exert a force on a charged particle which depends on the value of the charge, the particle's velocity, and the values of E and B at the location of the particle. The force is given by the Lorentz-force law

$$f = e(E + u \wedge B) \qquad [5]$$

in which e is the charge and u is the velocity. It is analogous to the gravitational force

$$f = mg \qquad [6]$$

on a particle of mass m in a gravitational field g. It is through the force law that an observer can, in principle, measure the electric and magnetic fields at a point, by measuring the force on a standard charge moving with known velocity.

Second, moving charges generate electric and magnetic fields. We shall not yet consider in detail the way in which they do this, beyond stating the following basic principles.

EM1. The fields depend linearly on the charges.

This means that if we superimpose two distributions of charge, then the resultant E and B fields are the sums of the respective fields that the two distributions generate separately.

EM2. A stationary point charge e generates an electric field, but no magnetic field. The electric field is given by

$$E = \frac{ker}{r^3} \qquad [7]$$

where r is the position vector from the charge, $r = |r|$, and k is a positive constant, analogous to the gravitational constant.

By combining [7] and [5], we obtain an inverse-square law electrostatic force

$$\frac{kee'}{r^2} \qquad [8]$$

between two stationary charges; unlike gravity, it is repulsive when the charges have the same sign.

EM3. A point charge moving with velocity v generates a magnetic field

$$B = \frac{k'ev \wedge r}{r^3} \qquad [9]$$

where k' is a second positive constant.

This is extrapolated from measurements of the magnetic field generated by currents flowing in electrical circuits.

The constants k and k' in EM2 and EM3 determine the strengths of electric and magnetic interactions. They are usually denoted by

$$k = \frac{1}{4\pi\epsilon_0}, \qquad k' = \frac{\mu_0}{4\pi} \qquad [10]$$

Charge e is measured in coulombs, $|B|$ in teslas, and $|E|$ in volts per meter. With other quantities in SI units,

$$\epsilon_0 = 8.9 \times 10^{-12}, \qquad \mu_0 = 1.3 \times 10^{-6} \qquad [11]$$

The charge of an electron is -1.6×10^{-19} C; the current through an electric fire is a flow of 5–10 C s^{-1}. The earth's magnetic field is about 4×10^{-5} T; a bar magnet's is about 1 T; there is a field of about 50 T on the second floor of the Clarendon Laboratory in Oxford; and the magnetic field on the surface of a neutron star is about 10^8 T.

Although we are more aware of gravity in everyday life, it is very much weaker than the electrostatic force – the electrostatic repulsion between two protons is a factor of 1.2×10^{36} greater than their gravitational attraction (at any separation, both forces obey the inverse-square law).

Our aim is to pass from EM1–EM3 to Maxwell's equations, by replacing [7] and [9] by partial differential equations that relate the field strengths to the charge and current densities ρ and J of a

continuous distribution of charge. The densities are defined as the limits

$$\rho = \lim_{V\to 0}\left(\frac{\sum e}{V}\right), \qquad \boldsymbol{J} = \lim_{V\to 0}\left(\frac{\sum e\boldsymbol{v}}{V}\right) \qquad [12]$$

where V is a small volume containing the point, e is a charge within the volume, and $\boldsymbol{v}$ is its velocity; the sums are over the charges in V and the limits are taken as the volume is shrunk (although we shall not worry too much about the precise details of the limiting process).

Stationary Distributions of Charge

We begin the task of converting the basic principles into partial differential equations by looking at the electric field of a stationary distribution of charge, where the passage to the continuous limit is made by using the Gauss theorem to restate the inverse-square law.

The Gauss theorem relates the integral of the electric field over a closed surface to the total charge contained within it. For a point charge, the electric field is given by EM2:

$$\boldsymbol{E} = \frac{e\boldsymbol{r}}{4\pi\epsilon_0 r^3}$$

Since $\operatorname{div}\boldsymbol{r} = 3$ and $\operatorname{grad} r = \boldsymbol{r}/r$, we have

$$\operatorname{div}(\boldsymbol{E}) = \operatorname{div}\left(\frac{e\boldsymbol{r}}{\pi\epsilon_0 r^3}\right) = \frac{e}{4\pi\epsilon_0}\left(\frac{3}{r^3} - \frac{3\boldsymbol{r}\cdot\boldsymbol{r}}{r^5}\right) = 0$$

everywhere except at $r = 0$. Therefore, by the divergence theorem,

$$\int_{\partial V} \boldsymbol{E}\cdot d\boldsymbol{S} = 0 \qquad [13]$$

for any closed surface ∂V bounding a volume V that does not contain the charge.

What if the volume does contain the charge? Consider the region bounded by the sphere S_R of radius R centered on the charge; S_R has outward unit normal $\boldsymbol{r}/r$. Therefore,

$$\int_{S_R} \boldsymbol{E}\cdot d\boldsymbol{S} = \frac{e}{4\pi R^2\epsilon_0}\int_{S_R} dS = \frac{e}{\epsilon_0}$$

In particular, the value of the surface integral on the left-hand side does not depend on R.

Now consider arbitrary finite volume bounded by a closed surface S. If the charge is not inside the volume, then the integral of $\boldsymbol{E}$ over S vanishes by [13]. If it is, then we can apply [13] to the volume V between S and a small sphere S_R to deduce that

$$\int_S \boldsymbol{E}\cdot d\boldsymbol{S} - \int_{S_R} \boldsymbol{E}\cdot d\boldsymbol{S} = \int_{\partial V} \boldsymbol{E}\cdot d\boldsymbol{S} = 0$$

and that the integrals of $\boldsymbol{E}$ over S and S_R are the same. Therefore,

$$\int_S \boldsymbol{E}\cdot d\boldsymbol{S} = \begin{cases} e/\epsilon_0 & \text{if the charge is in} \\ & \text{the volume bounded by } S \\ 0 & \text{otherwise} \end{cases}$$

When we sum over a distribution of charges, the integral on the left picks out the total charge within S. Therefore, we have the Gauss theorem.

The Gauss theorem. For any closed surface ∂V bounding a volume V,

$$\int_{\partial V} \boldsymbol{E}\cdot d\boldsymbol{S} = Q/\epsilon_0$$

where $\boldsymbol{E}$ is the total electric field and Q is the total charge within V.

Now we can pass to the continuous limit. Suppose that $\boldsymbol{E}$ is generated by a distribution of charges with density ρ (charge per unit volume). Then by the Gauss theorem,

$$\int_{\partial V} \boldsymbol{E}\cdot d\boldsymbol{S} = \frac{1}{\epsilon_0}\int_V \rho\, dV$$

for any volume V. But then, by the divergence theorem,

$$\int_V (\operatorname{div}\boldsymbol{E} - \rho/\epsilon_0)\, dV = 0$$

Since this holds for any volume V, it follows that

$$\operatorname{div}\boldsymbol{E} = \rho/\epsilon_0 \qquad [14]$$

By an argument in a similar spirit, we can also show that the electric field of a stationary distribution of charge is conservative in the sense that the total work done by the field when a charge is moved around a closed loop vanishes; that is,

$$\oint \boldsymbol{E}\cdot d\boldsymbol{s} = 0$$

for any closed path. This is equivalent to

$$\operatorname{curl}\boldsymbol{E} = 0 \qquad [15]$$

since, by Stokes' theorem,

$$\oint \boldsymbol{E}\cdot d\boldsymbol{s} = \int_S \operatorname{curl}\boldsymbol{E}\cdot d\boldsymbol{S}$$

where S is any surface spanning the path. This vanishes for every path and for every S if and only if [15] holds.

The field of a single stationary charge is conservative since

$$E = -\text{grad}\ \phi, \quad \phi = \frac{e}{4\pi\epsilon_0 r}$$

and therefore curl $E = 0$ since the curl of a gradient vanishes identically. For a continuous distribution, $E = -\text{grad}\ \phi$, where

$$\phi(\boldsymbol{r}) = \frac{1}{4\pi\epsilon_0}\int_{r'\in V}\frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}V' \qquad [16]$$

In the integral, $\boldsymbol{r}$ (the position of the point at which ϕ is evaluated) is fixed, and the integration is over the positions $\boldsymbol{r}'$ of the individual charges. In spite of the singularity at $\boldsymbol{r} = \boldsymbol{r}'$, the integral is well defined. So, [15] also holds for a continuous distribution of stationary charge.

The Divergence of the Magnetic Field

We can apply the same argument that established the Gauss theorem to the magnetic field of a slow-moving charge. Here,

$$\boldsymbol{B} = \frac{\mu_0 e\boldsymbol{v}\wedge\boldsymbol{r}}{4\pi r^3}$$

where $\boldsymbol{r}$ is the vector from the charge to the point at which the field is measured. Since $\boldsymbol{r}/r^3 = -\text{grad}(1/r)$, we have

$$\text{div}\left(\boldsymbol{v}\wedge\frac{\boldsymbol{r}}{r^3}\right) = \boldsymbol{v}\wedge\text{curl}\left(\text{grad}\,\frac{1}{r}\right) = 0$$

Therefore, div $\boldsymbol{B} = 0$ except at $\boldsymbol{r} = 0$, as in the case of the electric field. However, in the magnetic case, the integral of the field over a surface surrounding the charge also vanishes, since if S_R is a sphere of radius R centered on the charge, then

$$\int_{S_R}\boldsymbol{B}\cdot\mathrm{d}\boldsymbol{S} = \frac{\mu_0 e}{4\pi}\int_{S_R}\frac{\boldsymbol{v}\wedge\boldsymbol{r}}{r^3}\cdot\frac{\boldsymbol{r}}{r}\,\mathrm{d}S = 0$$

By the divergence theorem, the same is true for any surface surrounding the charge. We deduce that if magnetic fields are generated only by moving charges, then

$$\int_{\partial V}\boldsymbol{B}\cdot\mathrm{d}\boldsymbol{S} = 0$$

for any volume V, and hence that

$$\text{div}\,\boldsymbol{B} = 0 \qquad [17]$$

Of course, if there were free "magnetic poles" generating magnetic fields in the same way that charges generate electric fields, then this would not hold; there would be a "magnetic pole density" on the right-hand side, by analogy with the charge density in [14].

Inconsistency with Galilean Relativity

Our central concern is the compatibility of the laws of electromagnetism with the principle of relativity. As Einstein observed, simple electromagnetic interactions do indeed depend only on relative motion; the current induced in a conductor moving through the field of a magnet is the same as that generated in a stationary conductor when a magnet is moved past it with the same relative velocity (Einstein 1905). Unfortunately, this symmetry is not reflected in our basic principles. We very quickly come up against contradictions if we assume that they hold in every inertial frame of reference.

One emerges as follows. An observer O can measure the values of $\boldsymbol{B}$ and $\boldsymbol{E}$ at a point by measuring the force on a particle of standard charge, which is related to the velocity $\boldsymbol{v}$ of the charge by the Lorentz-force law,

$$\boldsymbol{f} = e(\boldsymbol{E} + \boldsymbol{v}\wedge\boldsymbol{B})$$

A second observer O′ moving relative to the first with velocity $\boldsymbol{v}$ will see the same force, but now acting on a particle at rest. He will therefore measure the electric field to be $\boldsymbol{E}' = \boldsymbol{f}/e$. We conclude that an observer moving with velocity $\boldsymbol{v}$ through a magnetic field $\boldsymbol{B}$ and an electric field $\boldsymbol{E}$ should see an electric field

$$\boldsymbol{E}' = \boldsymbol{E} + \boldsymbol{v}\wedge\boldsymbol{B} \qquad [18]$$

By interchanging the roles of the two observers, we should also have

$$\boldsymbol{E} = \boldsymbol{E}' - \boldsymbol{v}\wedge\boldsymbol{B}' \qquad [19]$$

where $\boldsymbol{B}'$ is the magnetic field measured by the second observer. If both are to hold, then $\boldsymbol{B} - \boldsymbol{B}'$ must be a scalar multiple of $\boldsymbol{v}$.

But this is incompatible with EM3; if the fields are those of a point charge at rest relative to the first observer, then $\boldsymbol{E}$ is given by [7], and

$$\boldsymbol{B} = 0$$

On the other hand, the second observer sees the field of a point charge moving with velocity $-\boldsymbol{v}$. Therefore,

$$\boldsymbol{B}' = -\frac{\mu_0 e\boldsymbol{v}\wedge\boldsymbol{r}}{4\pi r^3}$$

So $\boldsymbol{B} - \boldsymbol{B}'$ is orthogonal to $\boldsymbol{v}$, not parallel to it.

This conspicuous paradox is resolved, in part, by the realization that EM3 is not exact; it holds only when the velocities are small enough for the magnetic force between two particles to be negligible in comparison with the electrostatic force. If v is a typical velocity, then the condition is that $v^2\mu_0$

should be much less than $1/\epsilon_0$. That is, the velocities involved should be much less than

$$c = \frac{1}{\sqrt{\epsilon_0 \mu_0}} = 3 \times 10^8 \,\mathrm{m\,s^{-1}}$$

This, of course, is the velocity of light.

The Limits of Galilean Invariance

Our basic principles EM1–EM3 must now be seen to be approximations – they describe the interactions of particles and fields when the particles are moving relative to each other at speeds much less than that of light. To emphasize that we cannot expect, in particular, EM3 to hold for particles moving at speeds comparable with c, we must replace it by

EM3′. A charge moving with velocity $\boldsymbol{v}$, where $v \ll c$, generates a magnetic field

$$\boldsymbol{B} = \frac{\mu_0 e \boldsymbol{v} \wedge \boldsymbol{r}}{4\pi r^3} + O(v^2/c^2) \qquad [20]$$

The magnetic field of a system of charges in general motion satisfies

$$\operatorname{div} \boldsymbol{B} = 0 \qquad [21]$$

In the second part, we have retained [21] as a differential form of the statement that there are no free magnetic poles; the magnetic field is generated only by the motion of the charges. With this change, the theory is consistent with the principle of relativity, provided that we ignore terms of order v^2/c^2. The substitution of EM3′ for EM3 resolves the conspicuous paradox; the symmetry noted by Einstein between the current generated by the motion of the conductor in a magnetic field and by the motion of a magnet past a conductor is explained, provided that the velocities are much less than that of light.

The central problem remains however; the equations of electromagnetism are not invariant under a Galilean transformation with velocity comparable to c. The paradox is still there, but it is more subtle than it appeared to be at first. There are three possible ways out: (1) the noninvariance is real and has observable effects (necessarily of order v^2/c^2 or smaller); (2) Maxwell's theory is wrong; or (3) the Galilean transformation is wrong. Disconcertingly, it is the last path that physics has taken. But that is to jump ahead in the story. Our task is to complete the derivation of Maxwell's equations.

Faraday's Law of Induction

The magnetic field of a slow-moving charge will always be small in relation to its electric field (even when we replace $\boldsymbol{B}$ by $c\boldsymbol{B}$ to put it into the same units as $\boldsymbol{E}$). The magnetic fields generated by currents in electrical circuits are not, however, dominated by large electric fields. This is because the currents are created by the flow, at slow velocity, of electrons, while overall the matter in the wire is roughly electrically neutral, with the electric fields of the positively charged nuclei and negatively charged electrons canceling.

This is the physical context to keep in mind in the following deduction of Faraday's law of induction from Galilean invariance for velocities much less than c. The law relates the electromotive force or "voltage" around an electrical circuit to the rate of change of the magnetic field $\boldsymbol{B}$ over a surface spanning the circuit. In its differential form, the law becomes one of Maxwell's equations.

Suppose first that the fields are generated by charges all moving relative to a given inertial frame of reference R with the same velocity $\boldsymbol{v}$. Then in a second frame R' moving relative to R with velocity $\boldsymbol{v}$, there is a stationary distribution of charge. If the velocity is much less than that of light, then the electric field $\boldsymbol{E}'$ measured in R' is related to the electric and magnetic $\boldsymbol{E}$ and $\boldsymbol{B}$ measured in R by

$$\boldsymbol{E}' = \boldsymbol{E} + \boldsymbol{v} \wedge \boldsymbol{B}$$

Since the field measured in R' is that of a stationary distribution of charge, we have

$$\operatorname{curl} \boldsymbol{E}' = 0$$

In R, the charges are all moving with velocity $\boldsymbol{v}$, so their configuration looks exactly the same from the point $\boldsymbol{r}$ at time t as it does from the point $\boldsymbol{r} + \boldsymbol{v}\tau$ at time $t + \tau$. Therefore,

$$\boldsymbol{B}(\boldsymbol{r} + \boldsymbol{v}\tau, t + \tau) = \boldsymbol{B}(\boldsymbol{r}, t)$$
$$\boldsymbol{E}(\boldsymbol{r} + \boldsymbol{v}\tau, t + \tau) = \boldsymbol{E}(\boldsymbol{r}, t)$$

and hence by taking derivatives with respect to τ at $\tau = 0$,

$$\begin{aligned} \boldsymbol{v} \cdot \operatorname{grad} \boldsymbol{B} + \frac{\partial \boldsymbol{B}}{\partial t} &= 0 \\ \boldsymbol{v} \cdot \operatorname{grad} \boldsymbol{E} + \frac{\partial \boldsymbol{E}}{\partial t} &= 0 \end{aligned} \qquad [22]$$

So we must have

$$\begin{aligned} 0 &= \operatorname{curl} \boldsymbol{E}' \\ &= \operatorname{curl} \boldsymbol{E} + \operatorname{curl}(\boldsymbol{v} \wedge \boldsymbol{B}) \\ &= \operatorname{curl} \boldsymbol{E} + \boldsymbol{v} \operatorname{div} \boldsymbol{B} - \boldsymbol{v} \cdot \operatorname{grad} \boldsymbol{B} \\ &= \operatorname{curl} \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} \end{aligned} \qquad [23]$$

since $\operatorname{div} \boldsymbol{B} = 0$. It follows that

$$\operatorname{curl} \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0 \qquad [24]$$

Equation [24] is linear in $\boldsymbol{B}$ and $\boldsymbol{E}$; so by adding the magnetic and electric fields of different streams of charges moving relative to R with different velocities, we deduce that it holds generally for the electric and magnetic fields generated by moving charges.

Equation [24] encodes Faraday's law of electromagnetic induction, which describes how changing magnetic fields can generate currents. In the static case

$$\frac{\partial \boldsymbol{B}}{\partial t} = 0$$

and the equation reduces to $\operatorname{curl} \boldsymbol{E} = 0$ – the condition that the electrostatic field should be conservative; that is, it should do no net work when a charge is moved around a closed loop.

More generally, consider a wire loop in the shape of a closed curve γ. Let S be a fixed surface spanning γ. Then we can deduce from eqn [24] that

$$\begin{aligned} \oint_\gamma \boldsymbol{E} \cdot \mathrm{d}\boldsymbol{s} &= \int_S \operatorname{curl} \boldsymbol{E} \cdot \mathrm{d}\boldsymbol{S} \\ &= -\int_S \frac{\partial \boldsymbol{B}}{\partial t} \cdot \mathrm{d}\boldsymbol{S} \\ &= -\frac{\mathrm{d}}{\mathrm{d}t} \int_S (\boldsymbol{B} \cdot \mathrm{d}\boldsymbol{S}) \end{aligned} \qquad [25]$$

If the magnetic field is varying, so that the integral of $\boldsymbol{B}$ over S is not constant, then the integral of $\boldsymbol{E}$ around the loop will not be zero. There will be a nonzero electric field along the wire, which will exert a force on the electrons in the wire and cause a current to flow.

The quantity

$$\oint \boldsymbol{E} \cdot \mathrm{d}\boldsymbol{s}$$

which is measured in volts, is the work done by the electric field when a unit charge makes one circuit of the wire. It is called the electromotive force around the circuit. The integral is the magnetic flux linking the circuit. The relationship [25] between electromotive force and rate of change of magnetic flux is Faraday's law.

The Field of Charges in Uniform Motion

We can extract another of Maxwell's equations from this argument. By EM3′, a single charge e with velocity $\boldsymbol{v}$ generates an electric field $\boldsymbol{E}$ and a magnetic field

$$\boldsymbol{B} = \frac{\mu_0 e \boldsymbol{v} \wedge \boldsymbol{r}}{4\pi r^3} + O(v^2/c^2)$$

where $\boldsymbol{r}$ is the vector from the charge to the point at which the field is measured. In the frame of reference R' in which the charge is at rest, its electric field is

$$\boldsymbol{E}' = \frac{e\boldsymbol{r}}{4\pi\epsilon_0 r^3}$$

In the frame in which it is moving with velocity $\boldsymbol{v}$, $\boldsymbol{E} = \boldsymbol{E}' + O(v/c)$. Therefore,

$$c\boldsymbol{B} = \frac{\boldsymbol{v} \wedge \boldsymbol{E}'}{c} = \frac{\boldsymbol{v} \wedge \boldsymbol{E}}{c} + O\left(\frac{v^2}{c^2}\right)$$

By taking the curl of both sides, and dropping terms of order v^2/c^2,

$$\begin{aligned} \operatorname{curl}(c\boldsymbol{B}) &= \operatorname{curl}\left(\frac{\boldsymbol{v} \wedge \boldsymbol{E}}{c}\right) \\ &= \frac{1}{c}(\boldsymbol{v} \operatorname{div} \boldsymbol{E} - \boldsymbol{v} \cdot \operatorname{grad} \boldsymbol{E}) \end{aligned}$$

But

$$\operatorname{div} \boldsymbol{E} = \rho/\epsilon_0, \qquad \boldsymbol{v} \cdot \operatorname{grad} \boldsymbol{E} = -\frac{\partial \boldsymbol{E}}{\partial t}$$

by [22]. Therefore,

$$\operatorname{curl}(c\boldsymbol{B}) - \frac{1}{c}\frac{\partial \boldsymbol{E}}{\partial t} = \frac{1}{c\epsilon_0}\boldsymbol{J} = c\mu_0 \boldsymbol{J}$$

where $\boldsymbol{J} = \rho\boldsymbol{v}$. By summing over the separate particle velocities, we conclude that

$$\operatorname{curl} \boldsymbol{B} - \frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} = \mu_0 \boldsymbol{J}$$

holds for an arbitrary distribution of charges, provided that their velocities are much less than that of light.

Maxwell's Equations

The basic principles, together with the assumption of Galilean invariance for velocities much less than that of light, have allowed us to deduce that the electric and magnetic fields generated by a continuous distribution of moving charges in otherwise empty space satisfy

$$\operatorname{div} \boldsymbol{E} = \frac{\rho}{\epsilon_0} \qquad [26]$$

$$\operatorname{div} \boldsymbol{B} = 0 \qquad [27]$$

$$\operatorname{curl} \boldsymbol{B} - \frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} = \mu_0 \boldsymbol{J} \qquad [28]$$

$$\operatorname{curl} \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0 \qquad [29]$$

where ρ is the charge density, J is the current density, and $c^2 = 1/\epsilon_0\mu_0$. These are Maxwell's equations, the basis of modern electrodynamics. Together with the Lorentz-force law, they describe the dynamics of charges and electromagnetic fields.

We have arrived at them by considering how basic electromagnetic processes appear in moving frames of reference – an unsatisfactory route because we have seen on the way that the principles on which we based the derivation are incompatible with Galilean invariance for velocities comparable with that of light. Maxwell derived them by analyzing an elaborate mechanical model of electric and magnetic fields – as displacements in the luminiferous ether. That is also unsatisfactory because the model has long been abandoned. The reason that they are accepted today as the basis of theoretical and practical applications of electromagnetism has little to do with either argument. It is first that they are self-consistent, and second that they describe the behavior of real fields with unreasonable accuracy.

The Continuity Equation

It is not immediately obvious that the equations are self-consistent. Given ρ and J as functions of the coordinates and time, Maxwell's equations are two scalar and two vector equations in the unknown components of $\boldsymbol{E}$ and $\boldsymbol{B}$. That is, a total of eight equations for six unknowns – more equations than unknowns. Therefore, it is possible that they are in fact inconsistent.

If we take the divergence of eqn [29], then we obtain

$$\frac{\partial}{\partial t}(\text{div}\,\boldsymbol{B}) = 0$$

which is consistent with eqn [27]; so no problem arises here. However, by taking the divergence of eqn [28] and substituting from eqn [26], we get

$$\begin{aligned} 0 &= \text{div curl}\,\boldsymbol{B} \\ &= \frac{1}{c^2}\frac{\partial}{\partial t}(\text{div}\,\boldsymbol{E}) + \mu_0 \text{div}\,\boldsymbol{J} \\ &= \mu_0\left(\frac{\partial \rho}{\partial t} + \text{div}\,\boldsymbol{J}\right) \end{aligned}$$

This gives a contradiction unless

$$\frac{\partial \rho}{\partial t} + \text{div}\,\boldsymbol{J} = 0 \qquad [30]$$

So the choice of ρ and $\boldsymbol{J}$ is not unconstrained; they must be related by the continuity equation [30]. This holds for physically reasonable distributions of charge; it is a differential form of the statement that charges are neither created nor destroyed.

Conservation of Charge

To see the connection between the continuity equation and charge conservation, let us look at the total charge within a fixed V bounded by a surface S. If charge is conserved, then any increase or decrease in a short period of time must be exactly balanced by an inflow or outflow of charge across S.

Consider a small element $\mathrm{d}\boldsymbol{S}$ of S with outward unit normal and consider all the particles that have a particular charge e and a particular velocity $\boldsymbol{v}$ at time t. Suppose that there are σ of these per unit volume (σ is a function of position). Those that cross the surface element between t and $t + \delta t$ are those that at time t lie in the region of volume

$$|\boldsymbol{v} \cdot \boldsymbol{n}\,\mathrm{d}S\,\delta t|$$

shown in **Figure 1**. They contribute $e\sigma\boldsymbol{v} \cdot \mathrm{d}\boldsymbol{S}\delta t$ to the outflow of charge through the surface element. But the value of $\boldsymbol{J}$ at the surface element is the sum of $e\sigma\boldsymbol{v}$ over all possible values of $\boldsymbol{v}$ and e. By summing over $\boldsymbol{v}$, e, and the elements of the surface, therefore, and by passing to the limit of a continuous distribution, the total rate of outflow is

$$\int_S \boldsymbol{J} \cdot \mathrm{d}\boldsymbol{S}$$

Charge conservation implies that the rate of outflow should be equal to the rate of decrease in the total charge within V. That is,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V \rho\,\mathrm{d}V + \int_S \boldsymbol{J} \cdot \mathrm{d}\boldsymbol{S} = 0 \qquad [31]$$

By differentiating the first term under the integral sign and by applying the divergence theorem to the second integral,

$$\int_V \left(\frac{\partial \rho}{\partial t} + \text{div}\boldsymbol{J}\right)\mathrm{d}V = 0 \qquad [32]$$

If this is to hold for any choice of V, then ρ and $\boldsymbol{J}$ must satisfy the continuity equation. Conversely, the continuity equation implies charge conservation.

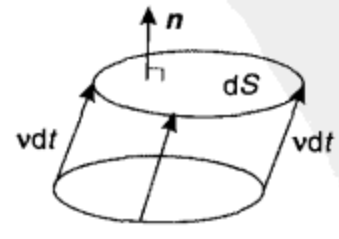

Figure 1 The outflow through a surface element.

The Displacement Current

The third of Maxwell's equations can be written as

$$\text{curl}\, \boldsymbol{B} = \mu_0 \left(\boldsymbol{J} + \epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} \right) \qquad [33]$$

in which form it can be read as an equation for an unknown magnetic field $\boldsymbol{B}$ in terms of a known current distribution $\boldsymbol{J}$ and electric field $\boldsymbol{E}$. When $\boldsymbol{E}$ and $\boldsymbol{J}$ are independent of t, it reduces to

$$\text{curl}\, \boldsymbol{B} = \mu_0 \boldsymbol{J}$$

which determines the magnetic field of a steady current, in a way that was already familiar to Maxwell's contemporaries. But his second term on the right-hand side of [33] was new; it adds to $\boldsymbol{J}$ the so-called vacuum displacement current

$$\epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t}$$

The name comes from an analogy with the behavior of charges in an insulating material. Here no steady current can flow, but the distribution of charges within the material is distorted by an external electric field. When the field changes, the distortion also changes, and the result appears as a current – the displacement current – which flows during the period of change. Maxwell's central insight was that the same term should be present even in empty space. The consequence was profound; it allowed him to explain the propagation of light as an electromagnetic phenomenon.

The Source-Free Equations

In a region of empty space, away from the charges generating the electric and magnetic fields, we have $\rho = 0 = \boldsymbol{J}$, and Maxwell's equations reduce to

$$\text{div}\, \boldsymbol{E} = 0 \qquad [34]$$

$$\text{div}\, \boldsymbol{B} = 0 \qquad [35]$$

$$\text{curl}\, \boldsymbol{B} - \frac{1}{c^2} \frac{\partial \boldsymbol{E}}{\partial t} = 0 \qquad [36]$$

$$\text{curl}\, \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0 \qquad [37]$$

where $c = 1/\sqrt{\epsilon_0 \mu_0}$. By taking the curl of eqn [36] and by substituting from eqns [35] and [37], we obtain

$$\begin{aligned} 0 &= \text{grad}\,(\text{div}\, \boldsymbol{B}) - \nabla^2 \boldsymbol{B} - \frac{1}{c^2} \text{curl} \left(\frac{\partial \boldsymbol{E}}{\partial t} \right) \\ &= -\nabla^2 \boldsymbol{B} - \frac{1}{c^2} \frac{\partial}{\partial t} (\text{curl}\, \boldsymbol{E}) \\ &= -\nabla^2 \boldsymbol{B} + \frac{1}{c^2} \frac{\partial^2 \boldsymbol{B}}{\partial t^2} \end{aligned} \qquad [38]$$

Therefore, the three components of $\boldsymbol{B}$ in empty space satisfy the (scalar) wave equation

$$\Box u = 0$$

Here $\Box$ is the d'Alembertian operator, defined by

$$\Box = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}$$

By taking the curl of eqn [37], we also obtain $\Box \boldsymbol{E} = 0$.

Monochromatic Plane Waves

The fact that $\boldsymbol{E}$ and $\boldsymbol{B}$ are vector-valued solutions of the wave equation in empty space suggests that we look for "plane wave" solutions of Maxwell's equations in which

$$\boldsymbol{E} = \boldsymbol{\alpha} \cos \Omega + \boldsymbol{\beta} \sin \Omega \qquad [39]$$

where $\boldsymbol{\alpha}, \boldsymbol{\beta}$ are constant vectors and

$$\Omega = \frac{\omega}{c} (ct - \boldsymbol{r} \cdot \boldsymbol{e}), \quad \boldsymbol{e} \cdot \boldsymbol{e} = 1 \qquad [40]$$

with $\omega > 0$, α, β, and $\boldsymbol{e}$ constant; ω is the frequency and $\boldsymbol{e}$ is a unit vector that gives the direction of propagation (adding τ to t and $c\tau \boldsymbol{e}$ to $\boldsymbol{r}$ leaves u unchanged). This satisfies the wave equation, but for a general choice of the constants, it will not be possible to find $\boldsymbol{B}$ such that eqns [34]–[37] also hold.

By taking the divergence of eqn [39], we obtain

$$\text{div}\, \boldsymbol{E} = \frac{\omega}{c} (\boldsymbol{e} \cdot \boldsymbol{\alpha} \sin \Omega - \boldsymbol{e} \cdot \boldsymbol{\beta} \cos \Omega) \qquad [41]$$

For eqn [34] to hold, therefore, we must choose $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ orthogonal to $\boldsymbol{e}$. For eqn [37] to hold, we must find $\boldsymbol{B}$ such that

$$\text{curl}\, \boldsymbol{E} = \frac{\omega}{c} (\boldsymbol{e} \wedge \boldsymbol{\alpha} \sin \Omega - \boldsymbol{e} \wedge \boldsymbol{\beta} \cos \Omega) = -\frac{\partial \boldsymbol{B}}{\partial t} \qquad [42]$$

A possible choice is

$$\boldsymbol{B} = \frac{\boldsymbol{e} \wedge \boldsymbol{E}}{c} = \frac{1}{c} (\boldsymbol{e} \wedge \boldsymbol{\alpha} \cos \Omega + \boldsymbol{e} \wedge \boldsymbol{\beta} \sin \Omega) \qquad [43]$$

and it is not hard to see that $\boldsymbol{E}$ and $\boldsymbol{B}$ then satisfy [35] and [36] as well.

The solutions obtained in this way are called "monochromatic electromagnetic plane waves."

Note that such waves are transverse in the sense that $\boldsymbol{E}$ and $\boldsymbol{B}$ are orthogonal to the direction of propagation. The definition $\boldsymbol{E}$ can be written more concisely in the form

$$\boldsymbol{E} = \mathrm{Re}\left[(\boldsymbol{\alpha} + \mathrm{i}\boldsymbol{\beta})\mathrm{e}^{-\mathrm{i}\Omega}\right] \qquad [44]$$

It is an exercise in Fourier analysis to show every solution in empty space is a combination of monochromatic plane waves. A plane wave has "plane" or "linear" polarization if $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are proportional. It has "circular" polarization if $\boldsymbol{\alpha}\cdot\boldsymbol{\alpha} = \boldsymbol{\beta}\cdot\boldsymbol{\beta}, \boldsymbol{\alpha}\cdot\boldsymbol{\beta} = 0$.

At the heart of Maxwell's theory was the idea that a light wave with definite frequency or color is represented by a monochromatic plane solution of his equations.

Potentials

For every solution of Maxwell's equations *in vacuo*, the components of $\boldsymbol{E}$ and $\boldsymbol{B}$ satisfy the three-dimensional wave equation; but the converse is not true. That is, it is not true in general that if

$$\Box\boldsymbol{B} = 0, \qquad \Box\boldsymbol{E} = 0$$

then $\boldsymbol{E}$ and $\boldsymbol{B}$ satisfy Maxwell's equations. For this to happen, the divergence of both fields must vanish, and they must be related by [36] and [37]. These additional constraints are somewhat simpler to handle if we work not with the fields themselves, but with auxiliary quantities called "potentials."

The definition of the potentials depends on standard integrability conditions from vector calculus. Suppose that $\boldsymbol{v}$ is a vector field, which may depend on time. If $\mathrm{curl}\,\boldsymbol{v} = 0$, then there exists a function ϕ such that

$$\boldsymbol{v} = \mathrm{grad}\,\phi \qquad [45]$$

If $\mathrm{div}\,\boldsymbol{v} = 0$, then there exists a second vector field $\boldsymbol{a}$ such that

$$\boldsymbol{v} = \mathrm{curl}\,\boldsymbol{a} \qquad [46]$$

Neither ϕ nor $\boldsymbol{a}$ is uniquely determined by $\boldsymbol{v}$. In the first case, if [45] holds, then it also holds when ϕ is replaced by $\phi' = \phi + f$, where f is a function of time alone; in the second, if [46] holds, then it also holds when $\boldsymbol{a}$ is replaced by

$$\boldsymbol{a}' = \boldsymbol{a} + \mathrm{grad}\,u$$

for any scalar function u of position and time. It should be kept in mind that the existence statements are local. If $\boldsymbol{v}$ is defined on a region U with nontrivial topology, then it may not be possible to find a suitable ϕ or $\boldsymbol{a}$ throughout the whole of U.

Suppose now that we are given fields $\boldsymbol{E}$ and $\boldsymbol{B}$ satisfying Maxwell's equations [26]–[29] with sources represented by the charge density ρ and the current density $\boldsymbol{J}$. Since $\mathrm{div}\,\boldsymbol{B} = 0$, there exists a time-dependent vector field $\boldsymbol{A}(t, x, y, z)$ such that

$$\boldsymbol{B} = \mathrm{curl}\,\boldsymbol{A}$$

If we substitute $\boldsymbol{B} = \mathrm{curl}\,\boldsymbol{A}$ into [29] and interchange curl with the time derivative, then we obtain

$$\mathrm{curl}\left(\boldsymbol{E} + \frac{\partial \boldsymbol{A}}{\partial t}\right) = 0$$

It follows that there exists a scalar $\phi(t, x, y, z)$ such that

$$\boldsymbol{E} = -\mathrm{grad}\,\phi - \frac{\partial \boldsymbol{A}}{\partial t} \qquad [47]$$

Such a vector field $\boldsymbol{A}$ is called a "magnetic vector potential"; a function ϕ such that eqn [47] holds is called an "electric scalar potential."

Conversely, given scalar and vector functions ϕ and $\boldsymbol{A}$ of t, x, y, z, we can define $\boldsymbol{B}$ and $\boldsymbol{E}$ by

$$\boldsymbol{B} = \mathrm{curl}\,\boldsymbol{A}, \qquad \boldsymbol{E} = -\mathrm{grad}\,\phi - \frac{\partial \boldsymbol{A}}{\partial t} \qquad [48]$$

Then two of Maxwell's equations hold automatically, since

$$\mathrm{div}\,\boldsymbol{B} = 0, \qquad \mathrm{curl}\,\boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0$$

The remaining pair translate into conditions on $\boldsymbol{A}$ and ϕ. Equation [26] becomes

$$\mathrm{div}\,\boldsymbol{E} = -\nabla^2\phi - \frac{\partial}{\partial t}(\mathrm{div}\,\boldsymbol{A}) = \frac{\rho}{\epsilon_0}$$

and eqn [28] becomes

$$\begin{aligned}\mathrm{curl}\,\boldsymbol{B} - \frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} &= -\nabla^2\boldsymbol{A} + \mathrm{grad}\ \mathrm{div}\,\boldsymbol{A} \\ &\quad + \frac{1}{c^2}\frac{\partial}{\partial t}\left(\mathrm{grad}\,\phi + \frac{\partial \boldsymbol{A}}{\partial t}\right) \\ &= \mu_0\boldsymbol{J}\end{aligned}$$

If we put

$$\alpha = \frac{1}{c^2}\frac{\partial \phi}{\partial t} + \mathrm{div}\,(\boldsymbol{A})$$

then we can rewrite the equations for $\boldsymbol{A}$ and ϕ more simply as

$$\Box\phi - \frac{\partial \alpha}{\partial t} = \frac{\rho}{\epsilon_0}$$

$$\Box\boldsymbol{A} + \mathrm{grad}\,\alpha = \mu_0\boldsymbol{J}$$

Here we have four equations (one scalar, one vector) in four unknowns (ϕ and the components of A). Any set of solutions ϕ, A determines a solution of Maxwell's equations via [48].

Gauge Transformations

Given solutions E and B of Maxwell's equations, what freedom is there in the choice of A and ϕ? First, A is determined by $\text{curl}\, A = B$ up to the replacement of A by

$$A' = A + \text{grad}\, u$$

for some function u of position and time. The scalar potential ϕ' corresponding to A' must be chosen so that

$$\begin{aligned} -\text{grad}\,\phi' &= E + \frac{\partial A'}{\partial t} \\ &= E + \frac{\partial A}{\partial t} + \text{grad}\left(\frac{\partial u}{\partial t}\right) \\ &= -\text{grad}\left(\phi - \frac{\partial u}{\partial t}\right) \end{aligned}$$

That is, $\phi' = \phi - \partial u/\partial t + f(t)$, where f is a function of t alone. We can absorb f into u by subtracting

$$\int f\, dt$$

(this does not alter A'). So the freedom in the choice of A and ϕ is to make the transformation

$$A \mapsto A' = A + \text{grad}\, u, \qquad \phi \mapsto \phi' = \phi - \frac{\partial u}{\partial t} \qquad [49]$$

for any $u = u(t, x, y, z)$. The transformation [49] is called a "gauge transformation."

Under [49],

$$\alpha \mapsto \alpha' = \frac{1}{c^2}\frac{\partial \phi'}{\partial t} + \text{div}(A') = \alpha - \Box u$$

It is possible to show, under certain very mild conditions on α, that the inhomogeneous wave equation

$$\Box u = \alpha \qquad [50]$$

has a solution $u = u(t, x, y, z)$. If we choose u so that [50] holds, then the transformed potentials A' and ϕ' satisfy

$$\text{div}(A') + \frac{1}{c^2}\frac{\partial \phi'}{\partial t} = 0$$

This is the "Lorenz gauge condition," named after L Lorenz (not the H A Lorentz of the "Lorentz contraction").

If we impose the Lorenz condition, then the only remaining freedom in the choice of A and ϕ is to make gauge transformations [49] in which u is a solution of the wave equation $\Box u = 0$. Under the Lorenz condition, Maxwell's equations take the form

$$\Box \phi = \rho/\epsilon_0, \qquad \Box A = \mu_0 J \qquad [51]$$

Consistency with the Lorenz condition follows from the continuity equation on ϕ and J.

In the absence of sources, therefore, Maxwell's equations for the potential in the Lorenz gauge reduce to

$$\Box \phi = 0, \qquad \Box A = 0 \qquad [52]$$

together with the constraint

$$\text{div}\, A + \frac{1}{c^2}\frac{\partial \phi}{\partial t} = 0$$

We can, for example, choose three arbitrary solutions of the scalar wave equation for the components of the vector potential, and then define ϕ by

$$\phi = c^2 \int \text{div}\, A dt$$

Whatever choice we make, we shall get a solution of Maxwell's equations, and every solution of Maxwell's equations (without sources) will arise from some such choice.

Historical Note

At the end of the eighteenth century, four types of electromagnetic phenomena were known, but not the connections between them.

- *Magnetism*, the word derives from the Greek for "stone from Magnesia."
- *Static electricity*, produced by rubbing amber with fur; the word "electricity" derives from the Greek for "amber."
- *Light*.
- *Galvanism* or "animal electricity" – the electricity produced by batteries, discovered by Luigi Galvani.

The construction of a unified theory was a slow and painful business. It was hindered by attempts, which seem bizarre in retrospect, to understand electromagnetism in terms of underlying mechanical models involving such inventions as "electric fluids" and "magnetic vortices." We can see the legacy of this period, which ended with Einstein's work in 1905, in the misleading and archaic terms that still survive in modern terminology: "magnetic flux," "lines of force," "electric displacement," and so on.

Maxwell's contribution was decisive, although much of what we now call "Maxwell's theory" is due to his successors (Lorentz, Hertz, Einstein, and so on); and, as we shall see, a key element in Maxwell's own description of electromagnetism – the "electromagnetic ether," an all-pervasive medium which was supposed to transmit electromagnetic waves – was thrown out by Einstein.

A rough chronology is as follows.

- 1800 Volta demonstrated the connection between galvanism and static electricity.
- 1820 Oersted showed that the current from a battery generates a force on a magnet.
- 1822 Ampère suggested that light was a wave motion in a "luminiferous ether" made up of two types of electric fluid. In the same year, Galileo's "Dialogue concerning the two chief world systems" was removed from the index of prohibited books.
- 1831 Faraday showed that moving magnets can induce currents.
- 1846 Faraday suggested that light is a vibration in magnetic lines of force.
- 1863 Maxwell published the equations that describe the dynamics of electric and magnetic fields.
- 1905 Einstein's paper "On the electrodynamics of moving bodies."

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Introductory Article: Equilibrium Statistical Mechanics

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Foundations: Atoms and Molecules

Classical statistical mechanics studies properties of macroscopic aggregates of particles, atoms, and molecules, based on the assumption that they are point masses subject to the laws of classical mechanics. Distinction between macroscopic and microscopic systems is evanescent and in fact the foundations of statistical mechanics have been laid on properties, proved or assumed, of few-particle systems.

Macroscopic systems are often considered in stationary states, which means that their microscopic configurations follow each other as time evolves while looking the same macroscopically. Observing time evolution is the same as sampling ("not too closely" time-wise) independent copies of the system prepared in the same way.

A basic distinction is necessary: a stationary state may or may not be in equilibrium. The first case arises when the particles are enclosed in a container Ω and are subject only to their mutual conservative interactions and, possibly, to external conservative forces: a typical example is a gas in a container subject to forces due to the walls of Ω and gravity, besides the internal interactions. This is a very restricted class of systems and states.

A more general case is when the system is in a stationary state but it is also subject to nonconservative forces: a typical example is a gas or fluid in which a wheel rotates, as in the Joule experiment, with some device acting to keep the temperature constant. The device is called a thermostat and in statistical mechanics it has to be modeled by forces, including nonconservative ones, which prevent an indefinite energy transfer from the external forcing to the system: such a transfer would impede the occurrence of stationary states. For instance, the thermostat could simply be a constant friction force (as in stirred incompressible liquids or as in electric wires in which current circulates because of an electromotive force).

A more fundamental approach would be to imagine that the thermostat device is not a phenomenologically introduced nonconservative force (e.g., a friction force) but is due to the interaction with an external infinite system which is in "equilibrium at infinity."

In any event nonequilibrium stationary states are intrinsically more complex than equilibrium states. Here attention will be confined to equilibrium

statistical mechanics of systems of N identical point particles $\mathbf{Q}=(q_1,\ldots,q_N)$ enclosed in a cubic box Ω, with volume V and side L, normally assumed to have perfectly reflecting walls.

Particles of mass m located at q,q' will be supposed to interact via a pair potential $\varphi(q-q')$. The microscopic motion follows the equations

$$m\ddot{q}_i = -\sum_{j=1}^{N}\partial_{q_i}\varphi(q_i-q_j)+\sum_i W_{\text{wall}}(q_i) \stackrel{\text{def}}{=} -\partial_{q_i}\Phi(\mathbf{Q}) \qquad [1]$$

where the potential φ is assumed to be smooth except, possibly, for $|q-q'|\le r_0$ where it could be $+\infty$, that is, the particles cannot come closer than r_0, and at r_0 [1] is interpreted by imagining that they undergo elastic collisions; the potential W_{wall} models the container and it will be replaced, unless explicitly stated, by an elastic collision rule.

The time evolution $(\mathbf{Q},\dot{\mathbf{Q}})\to S_t(\mathbf{Q},\dot{\mathbf{Q}})$ will, therefore, be described on the position – velocity space, $\widehat{\mathcal{F}}(N)$, of the N particles or, more conveniently, on the phase space, i.e., by a time evolution S_t on the momentum – position ($\mathbf{P},\mathbf{Q}$, with $\mathbf{P}=m\dot{\mathbf{Q}}$) space, $\mathcal{F}(N)$. The motion being conservative, the energy

$$U \stackrel{\text{def}}{=} \sum_i \frac{1}{2m}p_i^2+\sum_{i<j}\varphi(q_i-q_j)+\sum_i W_{\text{wall}}(q_i) \stackrel{\text{def}}{=} K(\mathbf{P})+\Phi(\mathbf{Q})$$

will be a constant of motion; the last term in Φ is missing if walls are perfect. This makes it convenient to regard the dynamics as associated with two dynamical systems $(\mathcal{F}(N),S_t)$ on the $6N$-dimensional phase space, and $(\mathcal{F}_U(N),S_t)$ on the $(6N-1)$-dimensional surface of energy U. Since the dynamics [1] is Hamiltonian on phase space, with Hamiltonian

$$H(\mathbf{P},\mathbf{Q}) \stackrel{\text{def}}{=} \sum_i \frac{1}{2m}p_i^2+\Phi(\mathbf{Q}) \stackrel{\text{def}}{=} K+\Phi$$

it follows that the volume $\mathrm{d}^{3N}\mathbf{P}\mathrm{d}^{3N}\mathbf{Q}$ is conserved (i.e., a region E has the same volume as S_tE) and also the area $\delta(H(\mathbf{P},\mathbf{Q})-U)\mathrm{d}^{3N}\mathbf{P}\mathrm{d}^{3N}\mathbf{Q}$ is conserved.

The above dynamical systems are well defined, i.e., S_t is a map on phase space globally defined for all $t\in(-\infty,\infty)$, when the interaction potential is bounded below: this is implied by the *a priori* bounds due to energy conservation. For gravitational or Coulomb interactions, much more has to be said, assumed, and done in order to even define the key quantities needed for a statistical theory of motion.

Although our world is three dimensional (or at least was so believed to be until recent revolutionary theories), it will be useful to consider also systems of particles in dimension $d\neq 3$: in this case the above $6N$ and $3N$ become, respectively, $2dN$ and dN. Systems with dimension $d=1,2$ are in fact sometimes very good models for thin filaments or thin films. For the same reason, it is often useful to imagine that space is discrete and particles can only be located on a lattice, for example, on $\mathbb{Z}^d$ (see the section "Lattice models").

The reader is referred to Gallavotti (1999) for more details.

Pressure, Temperature, and Kinetic Energy

The beginning was BERNOULLI's derivation of the perfect gas law via the identification of the *pressure* at *numerical density* ρ with the average momentum transferred per unit time to a surface element of area $\mathrm{d}S$ on the walls: that is, the average of the observable $2mv\rho v\,\mathrm{d}S$, with v the normal component of the velocity of the particles that undergo collisions with $\mathrm{d}S$. If $f(v)\mathrm{d}v$ is the distribution of the normal component of velocity and $f(\boldsymbol{v})\mathrm{d}^3\boldsymbol{v}\equiv\prod_i f(v_i)\mathrm{d}^3\boldsymbol{v}$, $\boldsymbol{v}=(v_1,v_2,v_3)$, is the total velocity distribution, the average of the momentum transferred is $p\mathrm{d}S$ given by

$$\mathrm{d}S\int_{v>0}2mv^2\rho f(v)\mathrm{d}v=\mathrm{d}S\int mv^2\rho f(v)\mathrm{d}v = \rho\frac{2}{3}\mathrm{d}S\int\frac{m}{2}\boldsymbol{v}^2 f(\boldsymbol{v})\mathrm{d}^3\boldsymbol{v}=\rho\frac{2}{3}\left\langle\frac{K}{N}\right\rangle\mathrm{d}S \qquad [2]$$

Furthermore $(2/3)\langle K/N\rangle$ was identified as proportional to the absolute temperature $\langle K/N\rangle \stackrel{\text{def}}{=} \text{const}\,(3/2)T$ which, with present-day notations, is written as $(2/3)\langle K/N\rangle = k_{\text{B}}T$. The constant k_{B} was (later) called Boltzmann's constant and it is the same for at least all perfect gases. Its independence on the particular nature of the gas is a consequence of *Avogadro's law* stating that equal volumes of gases at the same conditions of temperature and pressure contain equal number of molecules.

Proportionality between average kinetic energy and temperature via the universal constant k_{B} became in fact a fundamental assumption extending to all aggregates of particles gaseous or not, never challenged in all later works (until quantum mechanics, where this is no longer true, see the section "Quantum statistics".

For more details, we refer the reader to Gallavotti (1999).

Heat and Entropy

After Clausius' discovery of entropy, BOLTZMANN, in order to explain it mechanically, introduced the *heat theorem*, which he developed to full generality between 1866 and 1884. Together with the mentioned identification of absolute temperature with average kinetic energy, the heat theorem can also be considered a founding element of statistical mechanics.

The theorem makes precise the notion of time average and then states in great generality that given any mechanical system one can associate with its dynamics four quantities U, V, p, T, defined as time averages of suitable mechanical observables (i.e., functions on phase space), so that when the external conditions are infinitesimally varied and the quantities U, V change by $\mathrm{d}U, \mathrm{d}V$, respectively, the ratio $(\mathrm{d}U + p\mathrm{d}V)/T$ is exact, i.e., there is a function $S(U, V)$ whose corresponding variation equals the ratio. It will be better, for the purpose of considering very large boxes ($V \to \infty$) to write this relation in terms of intensive quantities $u \stackrel{\text{def}}{=} U/N$ and $v = V/N$ as

$$\frac{\mathrm{d}u + p\mathrm{d}v}{T} \text{ is exact} \qquad [3]$$

i.e., the ratio equals the variation $\mathrm{d}s$ of $s(U/N, V/N) \equiv (1/N)S(U, V)$.

The proof originally dealt with *monocyclic* systems, i.e., systems in which all motions are periodic. The assumption is clearly much too restrictive and justification for it developed from the early "nonperiodic motions can be regarded as periodic with infinite period" (1866), to the later *ergodic hypothesis* and finally to the realization that, after all, the heat theorem does not really depend on the ergodic hypothesis (1884).

Although for a one-dimensional system the proof of the heat theorem is a simple check, it was a real breakthrough because it led to an answer to the general question as to under which conditions one could define mechanical quantities whose variations were constrained to satisfy [3] and therefore could be interpreted as a mechanical model of Clausius' macroscopic thermodynamics. It is reproduced in the following.

Consider a one-dimensional system subject to forces with a confining potential $\varphi(x)$ such that $|\varphi'(x)| > 0$ for $|x| > 0, \varphi''(0) > 0$ and $\varphi(x) \underset{x \to \infty}{\longrightarrow} +\infty$. All motions are periodic, so that the system is monocyclic. Suppose that the potential $\varphi(x)$ depends on a parameter V and define a *state* to be a motion with given energy U and given V; let

$$\begin{aligned} U &= \text{total energy of the system} \equiv K + \Phi \\ T &= \text{time average of the kinetic energy } K = \langle K \rangle \\ V &= \text{the parameter on which } \varphi \\ &\quad \text{is supposed to depend} \\ p &= -\text{time average of } \partial_V \varphi, -\langle \partial_V \varphi \rangle \end{aligned} \qquad [4]$$

A state is thus parametrized by U, V. If such parameters change by $\mathrm{d}U, \mathrm{d}V$, respectively, and if $\mathrm{d}L \stackrel{\text{def}}{=} -p\mathrm{d}V, \mathrm{d}Q \stackrel{\text{def}}{=} \mathrm{d}U + p\mathrm{d}V$, then [3] holds. In fact, let $x_\pm(U, V)$ be the extremes of the oscillations of the motion with given U, V and define S as

$$S = 2 \log \int_{x_-(U,V)}^{x_+(U,V)} \sqrt{(U - \varphi(x))}\mathrm{d}x$$

$$\Rightarrow \mathrm{d}S = \frac{\int (\mathrm{d}U - \partial_V \varphi(x)\mathrm{d}V)(\mathrm{d}x/\sqrt{K})}{\int (\mathrm{d}x/\sqrt{K})K} \qquad [5]$$

Noting that $\mathrm{d}x/\sqrt{K} = \sqrt{2/m}\,\mathrm{d}t$, [3] follows because time averages are given by integrating with respect to $\mathrm{d}x/\sqrt{K}$ and dividing by the integral of $1/\sqrt{K}$.

For more details, the reader is referred to Boltzmann (1968b) and Gallavotti (1999).

Heat Theorem and Ergodic Hypothesis

Boltzmann tried to extend the result beyond the one-dimensional systems (e.g., to Keplerian motions, which are not monocyclic unless only motions with a fixed eccentricity are considered). However, the early statement that "aperiodic motions can be regarded as periodic with infinite period" is really the heart of the application of the heat theorem for monocyclic systems to the far more complex gas in a box.

Imagine that the gas container Ω is closed by a piston of section A located to the right of the origin at distance L and acting as a lid, so that the volume is $V = AL$. The microscopic model for the piston will be a potential $\overline{\varphi}(L - \xi)$ if $x = (\xi, \eta, \zeta)$ are the coordinates of a particle. The function $\overline{\varphi}(r)$ will vanish for $r > r_0$, for some $r_0 \ll L$, and diverge to $+\infty$ at $r = 0$. Thus, r_0 is the width of the layer near the piston where the force of the wall is felt by the particles that happen to be roaming there.

The contribution to the total potential energy Φ due to the walls is $W_{\text{wall}} = \sum_j \overline{\varphi}(L - \xi_j)$ and $\partial_V \overline{\varphi} = A^{-1} \partial_L \overline{\varphi}$; assuming monocyclicity, it is necessary to evaluate the time average of $\partial_L \Phi(x) = \partial_L W_{\text{wall}} \equiv -\sum_j \overline{\varphi}'(L - \xi_j)$. As time evolves, the particles x_j with ξ_j in the layer within r_0 of the wall will feel the force exercised by the wall and

bounce back. One particle in the layer will contribute to the average of $\partial_L \Phi(x)$ the amount

$$\frac{1}{\text{total time}} 2\int_{t_0}^{t_1} -\overline{\varphi}'(L-\xi_j)\mathrm{d}t \qquad [6]$$

if t_0 is the first instant when the point j enters the layer and t_1 is the instant when the ξ-component of the velocity vanishes "against the wall." Since $-\overline{\varphi}'(L-\xi_j)$ is the ξ-component of the force, the integral is $2m|\dot{\xi}_j|$ (by Newton's law), provided, of course, $\dot{\xi}_j > 0$.

Suppose that no collisions between particles occur while the particles travel within the range of the potential of the wall, i.e., the mean free path is much greater than the range of the potential $\overline{\varphi}$ defining the wall. The contribution of collisions to the average momentum transfer to the wall per unit time is therefore given by, see [2],

$$\int_{v>0} 2mv\, f(v)\rho_{\text{wall}} A v\, \mathrm{d}v$$

if $\rho_{\text{wall}}, f(v)$ are the average density near the wall and, respectively, the average fraction of particles with a velocity component normal to the wall between v and $v + \mathrm{d}v$. Here p, f are supposed to be independent of the point on the wall: this should be true up to corrections of size $o(A)$.

Thus, writing the average kinetic energy per particle and per velocity component, $\int (m/2)v^2 f(v)\mathrm{d}v$, as $(1/2)\beta^{-1}$ (cf. [2]) it follows that

$$p \overset{\text{def}}{=} -\langle \partial_V \Phi \rangle = \rho_{\text{wall}} \beta^{-1} \qquad [7]$$

has the physical interpretation of pressure. $(1/2)\beta^{-1}$ is the average kinetic energy per degree of freedom: hence, it is proportional to the absolute temperature T (cf. see the section "Pressure, temperature, and kinetic energy").

On the other hand, if motion on the energy surface takes place on a single periodic orbit, the quantity p in [7] is the right quantity that would make the heat theorem work; see [4]. Hence, regarding the trajectory on each energy surface as periodic (i.e., the system as monocyclic) leads to the heat theorem with p, U, V, T having the right physical interpretation corresponding to their appellations. This shows that monocyclic systems provide natural models of thermodynamic behavior.

Assuming that a chaotic system like a gas in a container of volume V will satisfy, for practical purposes, the above property, a quantity p can be defined such that $\mathrm{d}U + p\mathrm{d}V$ admits the inverse of the average kinetic energy $\langle K \rangle$ as an integrating factor and, furthermore, $p, U, V, \langle K \rangle$ have the physical interpretations of pressure, energy, volume, and (up to a proportionality factor) absolute temperature, respectively.

Boltzmann's conception of space (and time) as discrete allowed him to conceive the property that the energy surface is constituted by "points" all of which belong to a single trajectory: a property that would be impossible if the phase space was really a continuum. Regarding phase space as consisting of a finite number of "cells" of finite volume h^{dN}, for some $h > 0$ (rather than of a continuum of points), allowed him to think, without logical contradiction, that the energy surface consisted of a single trajectory and, hence, that motion was a cyclic permutation of its points (actually cells).

Furthermore, it implied that the time average of an observable $F(\boldsymbol{P}, \boldsymbol{Q})$ had to be identified with its average on the energy surface computed via the Liouville distribution

$$C^{-1}\int F(\boldsymbol{P}, \boldsymbol{Q})\delta(H(\boldsymbol{P}, \boldsymbol{Q}) - U)\mathrm{d}\boldsymbol{P}\,\mathrm{d}\boldsymbol{Q}$$

with

$$C = \int \delta(H(\boldsymbol{P}, \boldsymbol{Q}) - U)\mathrm{d}\boldsymbol{P}\,\mathrm{d}\boldsymbol{Q}$$

(the appropriate normalization factor): a property that was written symbolically

$$\frac{\mathrm{d}t}{T} = \frac{\mathrm{d}\boldsymbol{P}\,\mathrm{d}\boldsymbol{Q}}{\int \mathrm{d}\boldsymbol{P}\,\mathrm{d}\boldsymbol{Q}}$$

or

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T F(S_t(\boldsymbol{P}, \boldsymbol{Q}))\mathrm{d}t$$

$$= \frac{\int F(\boldsymbol{P}', \boldsymbol{Q}')\delta(H(\boldsymbol{P}', \boldsymbol{Q}') - U)\,\mathrm{d}\boldsymbol{P}'\mathrm{d}\boldsymbol{Q}'}{\int \delta(H(\boldsymbol{P}', \boldsymbol{Q}') - U)\,\mathrm{d}\boldsymbol{P}'\mathrm{d}\boldsymbol{Q}'} \qquad [8]$$

The validity of [8] for all (piecewise smooth) observables F and for all points of the energy surface, with the exception of a set of zero area, is called the ergodic hypothesis.

For more details, the reader is referred to Boltzmann (1968) and Gallavotti (1999).

Ensembles

Eventually Boltzmann in 1884 realized that the validity of the heat theorem for averages computed via the right-hand side (rhs) of [8] held independently of the ergodic hypothesis, that is, [8] was not necessary because the heat theorem (i.e., [3]) could also be derived under the only assumption that the averages involved in its formulation were computed

as averages over phase space with respect to the probability distribution on the rhs of [8].

Furthermore, if T was identified with the average kinetic energy, U with the average energy, and p with the average force per unit surface on the walls of the container Ω with volume V, the relation [3] held for a variety of families of probability distributions on phase space, besides [8]. Among these are:

1. The "microcanonical ensemble," which is the collection of probability distributions on the rhs of [8] parametrized by $u = U/N, v = V/N$ (energy and volume per particle),

$$\mu^{\mathrm{mc}}_{u,v}(\mathrm{d}\boldsymbol{P}\,\mathrm{d}\boldsymbol{Q}) = \frac{1}{Z_{\mathrm{mc}}(U,N,V)}\delta(H(\boldsymbol{P},\boldsymbol{Q})-U)\frac{\mathrm{d}\boldsymbol{P}\,\mathrm{d}\boldsymbol{Q}}{N!h^{dN}} \quad [9]$$

   where h is a constant with the dimensions of an action which, in the discrete representation of phase space mentioned in the previous section, can be taken such that h^{dN} equals the volume of the cells and, therefore, the integrals with respect to [9] can be interpreted as an (approximate) sum over the cells conceived as microscopic configurations of N indistinguishable particles (whence the $N!$).
2. The "canonical ensemble," which is the collection of probability distributions parametrized by $\beta, v = V/N$,

$$\mu^{\mathrm{c}}_{\beta,v}(\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q}) = \frac{1}{Z_{\mathrm{c}}(\beta,N,V)}\mathrm{e}^{-\beta H(\boldsymbol{P},\boldsymbol{Q})}\frac{\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q}}{N!h^{dN}} \quad [10]$$

   to which more ensembles can be added, such as the grand canonical ensemble (Gibbs).
3. The "grand canonical ensemble" which is the collection of probability distributions parameterized by β, λ and defined over the space $\mathcal{F}_{\mathrm{gc}} = \cup_{N=0}^{\infty}\mathcal{F}(N)$,

$$\mu^{\mathrm{gc}}_{\beta,\lambda}(\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q}) = \frac{1}{Z_{\mathrm{gc}}(\beta,\lambda,V)}\mathrm{e}^{\beta\lambda N-\beta H(\boldsymbol{P},\boldsymbol{Q})}\frac{\mathrm{d}\boldsymbol{P}\mathrm{d}\boldsymbol{Q}}{N!h^{dN}} \quad [11]$$

Hence, there are several different models of thermodynamics. The key tests for accepting them as real microscopic descriptions of macroscopic thermodynamics are as follows.

1. A correspondence between the macroscopic states of thermodynamic equilibrium and the elements of a collection of probability distributions on phase space can be established by identifying, on the one hand, macroscopic thermodynamic states with given values of the thermodynamic functions and, on the other, probability distributions attributing the same average values to the corresponding microscopic observables (i.e., whose averages have the interpretation of thermodynamic functions).
2. Once the correct correspondence between the elements of the different ensembles is established, that is, once the pairs $(u,v),(\beta,v),(\beta,\lambda)$ are so related to produce the same values for the averages $U, V, k_{\mathrm{B}}T \stackrel{\mathrm{def}}{=} \beta^{-1}, p|\partial\Omega|$ of

$$H(\boldsymbol{P},\boldsymbol{Q}), V, \frac{2K(\boldsymbol{P})}{3N}, \int\delta_{\partial\Omega}(\boldsymbol{q}_1)2m(\boldsymbol{v}_1\cdot\boldsymbol{n})^2\,\mathrm{d}\boldsymbol{q}_1 \quad [12]$$

   where $(\delta_{\partial\Omega}(\boldsymbol{q}_1)$ is a delta-function pinning $\boldsymbol{q}_1$ to the surface $\partial\Omega$), then the averages of all physically interesting observables *should coincide* at least in the thermodynamic limit, $\Omega\to\infty$. In this way, the elements μ of the considered collection of probability distributions can be identified with the states of macroscopic equilibrium of the system. The μ's depend on parameters and therefore they form an ensemble: each of them corresponds to a macroscopic equilibrium state whose thermodynamic functions are appropriate averages of microscopic observables and therefore are functions of the parameters identifying μ.

Remark The word "ensemble" is often used to indicate the individual probability distributions of what has been called here an ensemble. The meaning used here seems closer to the original sense in the 1884 paper of Boltzmann (in other words, often by "ensemble" one means that collection of the phase space points on which a given probability distribution is considered, and this does not seem to be the original sense).

For instance, in the case of the microcanonical distributions this means interpreting energy, volume, temperature, and pressure of the equilibrium state with specific energy u and specific volume v as proportional, through appropriate universal proportionality constants, to the integrals with respect to $\mu^{\mathrm{mc}}_{u,v}(\mathrm{d}\boldsymbol{P}\,\mathrm{d}\boldsymbol{Q})$ of the mechanical quantities in [12]. The averages of other thermodynamic observables in the state with specific energy u and specific volume v should be given by their integrals with respect to $\mu^{\mathrm{mc}}_{u,v}$.

Likewise, one can interpret energy, volume, temperature, and pressure of the equilibrium state with specific energy u and specific volume v as the averages of the mechanical quantities [12] with respect to the canonical distribution $\mu^{\mathrm{c}}_{\beta,v}(\mathrm{d}\boldsymbol{P}\,\mathrm{d}\boldsymbol{Q})$ which has average specific energy precisely u. The averages of other thermodynamic observables in the state with specific energy and volume u and v are

given by their integrals with respect to $\mu^c_{\beta,v}$. A similar definition can be given for the description of thermodynamic equilibria via the grand canonical distributions.

For more details, see Gibbs (1981) and Gallavotti (1999).

Equivalence of Ensembles

BOLTZMANN proved that, computing averages via the microcanonical or canonical distributions, the essential property [3] was satisfied when changes in their parameters (i.e., u, v or β, v, respectively) induced changes du and dv on energy and volume, respectively. He also proved that the function s, whose existence is implied by [3], was the same function once expressed as a function of u, v (or of any pair of thermodynamic parameters, e.g., of T, v or p, u). A close examination of Boltzmann's proof shows that the [3] holds exactly in the canonical ensemble and up to corrections tending to 0 as $\Omega \to \infty$ in the microcanonical ensemble. Identity of thermodynamic functions evaluated in the two ensembles holds, as a consequence, up to corrections of this order. In addition, Gibbs added that the same held for the grand canonical ensemble.

Of course, not every collection of stationary probability distributions on phase space would provide a model for thermodynamics: Boltzmann called "orthodic" the collections of stationary distributions which generated models of thermodynamics through the above-mentioned identification of its elements with macroscopic equilibrium states. The microcanonical, canonical, and the later grand canonical ensembles are the chief examples of orthodic ensembles. Boltzmann and Gibbs proved these ensembles to be not only orthodic but to generate the same thermodynamic functions, that is to generate the same thermodynamics.

This meant freedom from the analysis of the truth of the doubtful ergodic hypothesis (still unproved in any generality) or of the monocyclicity (manifestly false if understood literally rather than regarding the phase space as consisting of finitely many small, discrete cells), and allowed Gibbs to formulate the problem of statistical mechanics of equilibrium as follows.

Problem Study the properties of the collection of probability distributions constituting (any) one of the above ensembles.

However, by no means the three ensembles just introduced exhaust the class of orthodic ensembles producing the same models of thermodynamics in the limit of infinitely large systems. The wealth of ensembles with the orthodicity property, hence leading to equivalent mechanical models of thermodynamics, can be naturally interpreted in connection with the phenomenon of phase transition (see the section "Phase transitions and boundary conditions").

Clearly, the quoted results do not "prove" that thermodynamic equilibria "are" described by the microcanonical, canonical, or grand canonical ensembles. However, they certainly show that, for most systems, independently of the number of degrees of freedom, one can define quite unambiguously a mechanical model of thermodynamics establishing parameter-free, system-independent, physically important relations between thermodynamic quantities (e.g., $\partial_u(p(u,v)/T(u,v)) \equiv \partial_v(1/T(u,v))$, from [3]).

The ergodic hypothesis which was at the root of the mechanical theorems on heat and entropy cannot be taken as a justification of their validity. Naively one would expect that the time scale necessary to see an equilibrium attained, called recurrence time scale, would have to be at least the time that a phase space point takes to visit all possible microscopic states of given energy: hence, an explanation of why the necessarily enormous size of the recurrence time is not a problem becomes necessary.

In fact, the recurrence time can be estimated once the phase space is regarded as discrete: for the purpose of countering mounting criticism, Boltzmann assumed that momentum was discretized in units of $(2mk_BT)^{1/2}$ (i.e., the average momentum size) and space was discretized in units of $\rho^{-1/3}$ (i.e., the average spacing), implying a volume of cells h^{3N} with $h \stackrel{\text{def}}{=} \rho^{-1/3}(2mk_BT)^{1/2}$; then he calculated that, even with such a gross discretization, a cell representing a microscopic state of $1\,\text{cm}^3$ of hydrogen at normal condition would require a time (called "recurrence time") of the order of $\sim 10^{10^{19}}$ times the age of the Universe (!) to visit the entire energy surface. In fact, the phase space volume is $\Gamma = (\rho^{-3}N(2mk_BT)^{3/2})^N \equiv h^{3N}$ and the number of cells of volume h^{3N} is $\Gamma/(N!h^{3N}) \simeq e^{3N}$; and the time to visit all will be $e^{3N}\tau_0$, with τ_0 a typical atomic unit, e.g., $10^{-12}\,\text{s}$ – but $N = 10^{19}$. In this sense, the statement boldly made by young Boltzmann that "aperiodic motions can be regarded as periodic with infinite period" was even made quantitative.

The recurrence time is clearly so long to be irrelevant for all purposes: nevertheless, the correctness of the microscopic theory of thermodynamics can still rely on the microscopic dynamics once it is understood (as stressed by Boltzmann) that the reason why we observe approach to equilibrium, and equilibrium itself, over "human" timescales

(which are far shorter than the recurrence times) is due to the property that on most of the energy surface the (very few) observables whose averages yield macroscopic thermodynamic functions (namely pressure, temperature, energy, ...) *assume the same value* even if N is only very moderately large (of the order of 10^3 rather than 10^{19}). This implies that this value coincides with the average and therefore satisfies the heat theorem without any contradiction with the length of the recurrence time. The latter rather concerns the time needed to the *generic observable* to thermalize, that is, to reach its time average: the generic observable will indeed take a very long time to "thermalize" but no one will ever notice, because the generic observable (e.g., the position of a pre-identified particle) is not relevant for thermodynamics.

The word "proof" is not used in the mathematical sense so far in this article: the relevance of a mathematically rigorous analysis was widely realized only around the 1960s at the same time when the first numerical studies of the thermodynamic functions became possible and rigorous results were needed to check the correctness of various numerical simulations.

For more details, the reader is referred to Boltzmann (1968a, b) and Gallavotti (1999).

Thermodynamic Limit

Adopting Gibbs axiomatic point of view, it is interesting to see the path to be followed to achieve an equivalence proof of three ensembles introduced in the section "Heat theorem and ergodic hypothesis."

A preliminary step is to consider, given a cubic box Ω of volume $V = L^d$, the normalization factors $Z^{\mathrm{gc}}(\beta, \lambda, V)$, $Z^{\mathrm{c}}(\beta, N, V)$, and $Z^{\mathrm{mc}}(U, N, V)$ in [9], [10], and [11], respectively, and to check that the following thermodynamic limits exist:

$$\begin{aligned}
&\beta p_{\mathrm{gc}}(\beta, \lambda) \stackrel{\mathrm{def}}{=} \lim_{V\to\infty} \frac{1}{V} \log Z^{\mathrm{gc}}(\beta, \lambda, V) \\
&-\beta f_{\mathrm{c}}(\beta, \rho) \stackrel{\mathrm{def}}{=} \lim_{V\to\infty, \frac{N}{V}=\rho} \frac{1}{N} \log Z^{\mathrm{c}}(\beta, N, V) \\
&k_{\mathrm{B}}^{-1} s_{\mathrm{mc}}(u, \rho) \\
&\quad \stackrel{\mathrm{def}}{=} \lim_{V\to\infty, N/V=\rho,\, U/N=u} \frac{1}{N} \log Z^{\mathrm{mc}}(U, N, V)
\end{aligned} \qquad [13]$$

where the density $\rho \stackrel{\mathrm{def}}{=} v^{-1} \equiv N/V$ is used, instead of v, for later reference. The normalization factors play an important role because they have simple thermodynamic interpretation (see the next section): they are called grand canonical, canonical, and microcanonical partition functions, respectively.

Not surprisingly, assumptions on the interparticle potential $\varphi(q - q')$ are necessary to achieve an existence proof of the limits in [13]. The assumptions on φ are not only quite general but also have a clear physical meaning. They are

1. *stability*: that is, existence of a constant $B \geq 0$ such that $\sum_{i<j}^{N} \varphi(q_i - q_j) \geq -BN$ for all $N \geq 0$, $q_1, \ldots, q_N \in \mathbb{R}^d$, and
2. *temperedness*: that is, existence of constants ε_0, $R > 0$ such that $|\varphi(q - q')| < B|q - q'|^{-d-\varepsilon_0}$ for $|q - q'| > R$.

The assumptions are satisfied by essentially all microscopic interactions with the notable exceptions of the gravitational and Coulombic interactions, which require a separate treatment (and lead to somewhat different results on the thermodynamic behavior).

For instance, assumptions (1), (2) are satisfied if $\varphi(q)$ is $+\infty$ for $|q| < r_0$ and smooth for $|q| > r_0$, for some $r_0 \geq 0$, and furthermore $\varphi(q) > B_0|q|^{-(d+\varepsilon_0)}$ if $r_0 < |q| \leq R$, while for $|q| > R$ it is $|\varphi(q)| < B_1|q|^{-(d+\varepsilon_0)}$, for some $B_0, B_1, \varepsilon_0 > 0, R > r_0$. Briefly, φ is fast diverging at contact and fast approaching 0 at large distance. This is called a (generalized) Lennard–Jones potential. If $r_0 > 0$, φ is called a hard-core potential. If $B_1 = 0$, the potential is said to have finite range. (See Appendix 1 for physical implications of violations of the above stability and temperedness properties.) However, in the following, it will be necessary, both for simplicity and to contain the length of the exposition, to restrict consideration to the case $B_1 = 0$, i.e., to

$$\begin{aligned}
&\varphi(q) > B_0|q|^{-(d+\varepsilon_0)}, \quad r_0 < |q| \leq R, \\
&|\varphi(q)| \equiv 0, \quad |q| > R
\end{aligned} \qquad [14]$$

unless explicitly stated.

Assuming stability and temperedness, the existence of the limits in [13] can be mathematically proved: in Appendix 2, the proof of the first is analyzed to provide the simplest example of the technique. A remarkable property of the functions $\beta p_{\mathrm{gc}}(\beta, \lambda)$, $-\beta\rho f_{\mathrm{c}}(\beta, \rho)$, and $\rho s_{\mathrm{mc}}(u, \rho)$ is that they are convex functions: hence, they are continuous in the interior of their domains of definition and, at one variable fixed, are differentiable with respect to the other with at most countably many exceptions.

In the case of a potential without hard core ($\rho_{\max} = \infty$), $-\rho f_{\mathrm{c}}(\beta, \rho)$ can be checked to tend to 0 slower than ρ as $\rho \to 0$, and to $-\infty$ faster than $-\rho$ as $\rho \to \infty$ (essentially proportionally to $-\rho \log \rho$ in both cases). Likewise, in the same case, $s_{\mathrm{mc}}(u, \rho)$ can be shown to tend to 0 slower than $u - u_{\min}$ as $u \to u_{\min}$, and to $-\infty$ faster than $-u$ as $u \to \infty$. The latter

asymptotic properties can be exploited to derive, from the relations between the partition functions in [13],

$$Z^{gc}(\beta,\lambda,V)=\sum_{N=0}^{\infty}e^{\beta\lambda N}Z^{c}(\beta,N,V)$$
$$Z^{c}(\beta,N,V)=\int_{-B}^{\infty}e^{-\beta U}Z^{mc}(U,N,V)\,dU \qquad [15]$$

and, from the above-mentioned convexity, the consequences

$$\beta p_{mc}(\beta,\lambda)=\max_{v}(\beta\lambda v^{-1}-\beta v^{-1}f_{c}(\beta,v^{-1}))$$
$$-\beta f_{c}(\beta,v^{-1})=\max_{u}(-\beta u+k_{B}^{-1}s_{mc}(u,v^{-1})) \qquad [16]$$

and that the maxima are attained in points, or intervals, internal to the intervals of definition. Let v_{gc}, u_{c} be points where the maxima are, respectively, attained in [16].

Note that the quantity $e^{\beta\lambda N}Z^{c}(\beta,N,V)/Z^{gc}(\beta,\lambda,V)$ has the interpretation of probability of a density $v^{-1}=N/V$ evaluated in the grand canonical distribution. It follows that, if the maximum in the first of [16] is strict, that is, it is reached at a single point, the values of v^{-1} in closed intervals not containing the maximum point v_{gc}^{-1} have a probability behaving as $<e^{-cV}$, $c>0$, as $V\to\infty$, compared to the probability of v^{-1}'s in any interval containing v_{gc}^{-1}. Hence, v_{gc} has the interpretation of average value of v in the grand canonical distribution, in the limit $V\to\infty$.

Likewise, the interpretation of

$$e^{-\beta uN}Z^{mc}(uN,N,V)/Z^{c}(\beta,N,V)$$

as probability in the canonical distribution of an energy density u shows that, if the maximum in the second of [16] is strict, the values of u in closed intervals not containing the maximum point u_{c} have a probability behaving as $<e^{-cV}, c>0$, as $V\to\infty$, compared to the probability of u's in any interval containing u_{c}. Hence, in the limit $\Omega\to\infty$, the average value of u in the canonical distribution is u_{c}.

If the maxima are strict, [16] also establishes a relation between the grand canonical density, the canonical free energy and the grand canonical parameter λ, or between the canonical energy, the microcanonical entropy, and the canonical parameter β:

$$\lambda=\partial_{v^{-1}}(v_{gc}^{-1}f_{c}(\beta,v_{gc}^{-1})),\qquad k_{B}\beta=\partial_{u}s_{mc}(u_{c},v^{-1}) \qquad [17]$$

where convexity and strictness of the maxima imply the derivatives existence.

Remark Therefore, in the equivalence between canonical and microcanonical ensembles, the canonical distribution with parameters (β,v) should correspond with the microcanonical with parameters (u_{c},v). The grand canonical distribution with parameters (β,λ) should correspond with the canonical with parameters (β,v_{gc}).

For more details, the reader is referred to Ruelle (1969) and Gallavotti (1999).

Physical Interpretation of Thermodynamic Functions

The existence of the limits [13] implies several properties of interest. The first is the possibility of finding the physical meaning of the functions p_{gc}, f_{c}, s_{mc} and of the parameters λ,β

Note first that, for all V the grand canonical average $\langle K\rangle_{\beta,\lambda}$ is $(d/2)\beta^{-1}\langle N\rangle_{\beta,\lambda}$ so that β^{-1} is proportional to the temperature $T_{gc}=T(\beta,\lambda)$ in the grand canonical distribution: $\beta^{-1}=k_{B}T(\beta,\lambda)$. Proceeding heuristically, the physical meaning of $p(\beta,\lambda)$ and λ can be found through the following remarks.

Consider the microcanonical distribution $\mu_{u,v}^{mc}$ and denote by $\int^{*}$ the integral over $(\boldsymbol{P},\boldsymbol{Q})$ extended to the domain of the $(\boldsymbol{P},\boldsymbol{Q})$ such that $H(\boldsymbol{P},\boldsymbol{Q})=U$ and, at the same time, $q_{1}\in dV$, where dV is an infinitesimal volume surrounding the region Ω. Then, by the microscopic definition of the pressure p (see the introductory section), it is

$$p\,dV=\frac{N}{Z(U,N,V)}\int^{*}\delta\frac{2}{3}\frac{p_{1}^{2}}{2m}\frac{d\boldsymbol{P}\,d\boldsymbol{Q}}{N!h^{dN}}$$
$$\equiv\frac{2}{3Z(U,N,V)}\int^{*}\delta K(\boldsymbol{P})\frac{d\boldsymbol{P}\,d\boldsymbol{Q}}{N!h^{dN}} \qquad [18]$$

where $\delta\equiv\delta(H(\boldsymbol{P},\boldsymbol{Q})-U)$. The RHS of [18] can be compared with

$$\frac{\partial_{V}Z(U,N,V)dV}{Z(U,N,V)}=\frac{N}{Z(U,N,V)}\int^{*}\frac{d\boldsymbol{P}\,d\boldsymbol{Q}}{N!h^{dN}}$$

to give

$$\frac{\partial_{V}Z\,dV}{Z}=N\frac{p\,dV}{(2/3)\langle K\rangle^{*}}=\beta p\,dV$$

because $\langle K\rangle^{*}$, which denotes the average $\int^{*}K/\int^{*}1$, should be essentially the same as the microcanonical average $\langle K\rangle_{mc}$ (i.e., insensitive to the fact that one particle is constrained to the volume dV) if N is large. In the limit $V\to\infty, V/N=v$, the latter remark together with the second of [17] yields

$$k_{B}^{-1}\partial_{v}s_{mc}(u,v^{-1})=\beta p(u,v),$$
$$k_{B}^{-1}\partial_{u}s_{mc}(u,v)=\beta \qquad [19]$$

respectively. Note that $p\geq 0$ and it is not increasing in v because $s_{mc}(\rho)$ is concave as a function of $v=\rho^{-1}$ (in fact, by the remark following [14] $\rho s_{mc}(u,\rho)$ is convex in ρ and, in general, if $\rho g(\rho)$ is convex in ρ then $g(v^{-1})$ is always concave in $v=\rho^{-1}$).

Hence, $ds_{mc}(u,v) = (du + pdv)/T$, so that taking into account the physical meaning of p, T (as pressure and temperature, see the section "Pressure, temperature, and kinetic energy"), s_{mc} is, in thermodynamics, the entropy. Therefore (see the second of [16]), $-\beta f_c(\beta,\rho) = -\beta u_c + k_B^{-1} s_{mc}(u_c,\rho)$ becomes

$$f_c(\beta,\rho) = u_c - T_c s_{mc}(u_c,\rho),$$
$$df_c = -p\,dv - s_{mc}\,dT \qquad [20]$$

and since u_c has the interpretation (as mentioned in the last section) of average energy in the canonical distribution $\mu^c_{\beta,v}$ it follows that f_c has the thermodynamic interpretation of free energy (once compared with the definition of free energy, $F = U - TS$, in thermodynamics).

By [17] and [20],

$$\lambda = \partial_{v^{-1}}(v_{gc}^{-1} f_c(\beta, v_{gc}^{-1})) \equiv u_c - T_c s_{mc} + p v_{gc}$$

and v_{gc} has the meaning of specific volume v. Hence, after comparison with the definition of chemical potential, $\lambda V = U - TS + pV$, in thermodynamics, it follows that the thermodynamic interpretation of λ is the chemical potential and (see [16], [17]), the grand canonical relation

$$\beta p_{gc}(\beta,\lambda) = \beta\lambda v_{gc}^{-1} - \beta v_{gc}^{-1}(-\beta u_c + k_B^{-1} s_{mc}(u_c, v^{-1}))$$

shows that $p_{gc}(\beta,\lambda) \equiv p$, implying that $p_{gc}(\beta,\lambda)$ is the pressure expressed, however, as a function of temperature and chemical potential.

To go beyond the heuristic derivations above, it should be remarked that convexity and the property that the maxima in [16], [17] are reached in the interior of the intervals of variability of v or u are sufficient to turn the above arguments into rigorous mathematical deductions: this means that given [19] as definitions of $p(u,v), \beta(u,v)$, the second of [20] follows as well as $p_{gc}(\beta,\lambda) \equiv p(u_v, v_{gc}^{-1})$. But the values v_{gc} and u_c in [16] are not necessarily unique: convex functions can contain horizontal segments and therefore the general conclusion is that the maxima may possibly be attained in intervals. Hence, instead of a single v_{gc}, there might be a whole interval $[v_-, v_+]$, where the rhs of [16] reaches the maximum and, instead of a single u_c, there might be a whole interval $[u_-, u_+]$ where the rhs of [17] reaches the maximum.

Convexity implies that the values of λ or β for which the maxima in [16] or [17] are attained in intervals rather than in single points are rare (i.e., at most denumerably many): the interpretation is, in such cases, that the thermodynamic functions show discontinuities, and the corresponding phenomena are called phase transitions (see the next section).

For more details the reader is referred to Ruelle (1969) and Gallavotti (1999).

Phase Transitions and Boundary Conditions

The analysis in the last two sections of the relations between elements of ensembles of distributions describing macroscopic equilibrium states not only allows us to obtain mechanical models of thermodynamics but also shows that the models, for a given system, coincide at least as $\Omega \to \infty$. Furthermore, the equivalence between the thermodynamic functions computed via corresponding distributions in different ensembles can be extended to a full equivalence of the distributions.

If the maxima in [16] are attained at single points v_{gc} or u_c the equivalence should take place in the sense that a correspondence between $\mu^{gc}_{\beta,\lambda}, \mu^c_{\beta,v}, \mu^{mc}_{u,v}$ can be established so that, given any local observable $F(P,Q)$, defined as an observable depending on (P,Q) only through the p_i, q_i with $q_i \in \Lambda$, where $\Lambda \subset \Omega$ is a finite region, has the same average with respect to corresponding distributions in the limit $\Omega \to \infty$.

The correspondence is established by considering $(\lambda,\beta) \leftrightarrow (\beta, v_{gc}) \leftrightarrow (u_{mc}, v)$, where v_{gc} is where the maximum in [16] is attained, $u_{mc} \equiv u_c$ is where the maximum in [17] is attained and $v_{gc} \equiv v$, (cf. also [19], [20]). This means that the limits

$$\lim_{V\to\infty} \int F(P,Q)\mu^a(dP\,dQ) \stackrel{\text{def}}{=} \langle F\rangle_a$$
$$(a - \text{independent}),\ a = gc, c, mc \qquad [21]$$

coincide if the averages are evaluated by the distributions $\mu^{gc}_{\beta,\lambda}, \mu^c_{\beta,v_c}, \mu^{mc}_{u_{mc},v_{mc}}$

Exceptions to [21] are possible: and are certainly likely to occur at values of u, v where the maxima in [16] or [17] are attained in intervals rather than in isolated points; but this does not exhaust, in general, the cases in which [21] may not hold.

However, no case in which [21] fails has to be regarded as an exception. It rather signals that an interesting and important phenomenon occurs. To understand it properly, it is necessary to realize that the grand canonical, canonical, and microcanonical families of probability distributions are by far not the only ensembles of probability distributions whose elements can be considered to generate models of thermodynamics, that is, which are orthodic in the sense of the discussion in the section "Equivalence of ensembles." More general families of orthodic statistical ensembles of probability

distributions can be very easily conceived. In particular:

Definition Consider the grand canonical, canonical, and microcanonical distributions associated with an energy function in which the potential energy contains, besides the interaction Φ between particles located inside the container, also the interaction energy $\Phi_{\text{in,out}}$ between particles inside the container and external particles, identical to the ones in the container but not allowed to move and fixed in positions such that in every unit cube Δ external to Ω there is a finite number of them bounded independently of Δ. Such configurations of external particles will be called "boundary conditions of fixed external particles."

The thermodynamic limit with such boundary conditions is obtained by considering the grand canonical, canonical, and microcanonical distributions constructed with potential energy function $\Phi + \Phi_{\text{in,out}}$ in containers Ω of increasing size taking care that, while the size increases, the fixed particles that would become internal to Ω are eliminated. The argument used in the section "Thermodynamic limit" to show that the three models of thermodynamics, considered there, did define the same thermodynamic functions can be repeated to reach the conclusion that also the (infinitely many) "new" models of thermodynamics in fact give rise to the same thermodynamic functions and averages of local observables. Furthermore, the values of the limits corresponding to [13] can be computed using the new partition functions and coincide with the ones in [13] (i.e., they are independent of the boundary conditions).

However, it may happen, and in general it is the case, for many models and for particular values of the state parameters, that the limits in [21] do not coincide with the analogous limits computed in the new ensembles, that is, the averages of some local observables are unstable with respect to changes of boundary conditions with fixed particles.

There is a very natural interpretation of such apparent ambiguity of the various models of thermodynamics: namely, at the values of the parameters that are selected to describe the macroscopic states under consideration, there may correspond different equilibrium states with the same parameters. When the maximum in [16] is reached on an interval of densities, one should not think of any failure of the microscopic models for thermodynamics: rather one has to think that there are several states possible with the same β, λ and that they can be identified with the probability distributions obtained by forming the grand canonical, canonical, or microcanonical distributions with different kinds of boundary conditions.

For instance, a boundary condition with high density may produce an equilibrium state with parameters β, λ which also has high density, i.e., the density v_+^{-1} at the right extreme of the interval in which the maximum in [16] is attained, while using a low-density boundary condition the limit in [21] may describe the averages taken in a state with density v_-^{-1} at the left extreme of the interval or, perhaps, with a density intermediate between the two extremes. Therefore, the following definition emerges.

Definition If the grand canonical distributions with parameters (β, λ) and different choices of fixed external particles boundary conditions generate for some local observable F average values which are different by more than a quantity $\delta > 0$ for all large enough volumes Ω then one says that the system has a phase transition at (β, λ). This implies that the limits in [21], when existing, will depend on the boundary condition and their values will represent averages of the observables in "different phases." A corresponding definition is given in the case of the canonical and microcanonical distributions when, given (β, v) or (u, v), the limit in [21] depends on the boundary conditions for some F.

Remarks

1. The idea is that by fixing one of the thermodynamic ensembles and by varying the boundary conditions one can realize all possible states of equilibrium of the system that can exist with the given values of the parameters determining the state in the chosen ensemble (i.e., (β, λ), (β, v), or (u, v) in the grand canonical, canonical, or microcanonical cases, respectively).
2. The impression that in order to define a phase transition the thermodynamic limit is necessary is incorrect: the definition does not require considering the limit $\Omega \to \infty$. The phenomenon that occurs is that by changing boundary conditions the average of a local observable can change at least by amounts independent of the system size. Hence, occurrence of a phase transition is perfectly observable in finite volume: it suffices to check that by changing boundary conditions the average of some observable changes by an amount whose minimal size is volume independent. It is a manifestation of an instability of the averages with respect to changes in boundary conditions: an instability which does not fade away when the boundary recedes to infinity, i.e., boundary perturbations produce

bulk effects and at a phase transition the averages of the local observable, if existing at all, will exhibit a nontrivial dependence on the boundary conditions. This is also called "long range order."

3. It is possible to show that when this happens then some thermodynamic function whose value is independent of the boundary condition (e.g., the free energy in the canonical distributions) has discontinuous derivatives in terms of the parameters of the ensemble. This is in fact one of the frequently-used alternative definitions of phase transitions: the latter two natural definitions of first-order phase transition are equivalent. However, it is very difficult to prove that a given system shows a phase transition. For instance, existence of a liquid–gas phase transition is still an open problem in systems of the type considered until the section "Lattice models" below.
4. A remarkable unification of the theory of the equilibrium ensembles emerges: all distributions of any ensemble describe equilibrium states. If a boundary condition is fixed once and for all, then some equilibrium states might fail to be described by an element of an ensemble. However, if all boundary conditions are allowed then all equilibrium states should be realizable in a given ensemble by varying the boundary conditions.
5. The analysis leads us to consider as completely equivalent without exceptions grand canonical, canonical, or microcanonical ensembles enlarged by adding to them the distributions with potential energy augmented by the interaction with fixed external particles.
6. The above picture is really proved only for special classes of models (typically in models in which particles are constrained to occupy points of a lattice and in systems with hard core interactions, $r_0 > 0$ in [14]) but it is believed to be correct in general. At least it is consistent with all that is known so far in classical statistical mechanics. The difficulty is that, conceivably, one might even need boundary conditions more complicated than the fixed particles boundary conditions (e.g., putting different particles outside, interacting with the system with an arbitrary potential, rather than via φ).

The discussion of the equivalence of the ensembles and the question of the importance of boundary conditions has already imposed the consideration of several limits as $\Omega \to \infty$. Occasionally, it will again come up. For conciseness, it is useful to set up a formal definition of equilibrium states of an infinite-volume system: although infinite volume is an idealization void of physical reality, it is nevertheless useful to define such states because certain notions (e.g., that of pure state) can be sharply defined, with few words and avoiding wide circumvolutions, in terms of them. Therefore, let:

Definition An infinite-volume state with parameters (β, v), (u, v) or (β, λ) is a collection of average values $F \to \langle F \rangle$ obtained, respectively, as limits of finite-volume averages $\langle F \rangle_{\Omega_n}$ defined from canonical, microcanonical, or grand canonical distributions in Ω_n with fixed parameters (β, v), (u, v) or (β, λ) and with general boundary condition of fixed external particles, on sequences $\Omega_n \to \infty$ for which such limits exist simultaneously for all local observables F.

Having set the definition of infinite-volume state consider a local observable $G(X)$ and let $\tau_\xi G(X) = G(X + \xi), \xi \in \mathbb{R}^d$, with $X + \xi$ denoting the configuration X in which all particles are translated by ξ: then an infinite-volume state is called a pure state if for any pair of local observables F, G it is

$$\langle F \tau_\xi G \rangle - \langle F \rangle \langle \tau_\xi G \rangle \underset{\xi \to \infty}{\longrightarrow} 0 \qquad [22]$$

which is called a cluster property of the pair F, G.

The result alluded to in remark (6) is that at least in the case of hard-core systems (or of the simple lattice systems discussed in the section "Lattice models") the infinite-volume equilibrium states in the above sense exhaust at least the totality of the infinite-volume pure states. Furthermore, the other states that can be obtained in the same way are convex combinations of the pure states, i.e., they are "statistical mixtures" of pure phases. Note that $\langle \tau_\xi G \rangle$ cannot be replaced, in general, by $\langle G \rangle$ because not all infinite-volume states are necessarily translation invariant and in simple cases (e.g., crystals) it is even possible that no translation-invariant state is a pure state.

Remarks

1. This means that, in the latter models, generalizing the boundary conditions, for example considering external particles to be not identical to the ones inside the system, using periodic or partially periodic boundary conditions, or the widely used alternative of introducing a small auxiliary potential and first taking the infinite-volume states in presence of it and then letting the potential vanish, does not enlarge further the set of states (but may sometimes be useful: an example of a study of a phase transition by using the latter method of small fields will be given in the section "Continuous symmetries: 'no $d = 2$ crystal' theorem").

2. If χ is the indicator function of a local event, it will make sense to consider the probability of occurrence of the event in an infinite-volume state defining it as $\langle\chi\rangle$. In particular, the probability density for finding p particles at $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_p$, called the p-point correlation function, will thus be defined in an infinite-volume state. For instance, if the state is obtained as a limit of canonical states $\langle\cdot\rangle_{\Omega_n}$ with parameters $\beta, \rho, \rho = N_n/V_n$, in a sequence of containers Ω_n, then

$$\rho(\boldsymbol{x}) = \lim_n \left\langle \sum_{j=1}^{N_n} \delta(\boldsymbol{x} - \boldsymbol{q}_j) \right\rangle_{\Omega_n}$$

$$\rho(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_p) = \lim_n \left\langle \sum_{i_1,\ldots,i_p}^{N_n} \prod_{j=1}^{p} \delta(\boldsymbol{x}_j - \boldsymbol{q}_{i_j}) \right\rangle_{\Omega_n}$$

where the sum is over the ordered p-ples $(j_1, \ldots, j_p)$. Thus, the *pair correlation* $\rho(\boldsymbol{q}, \boldsymbol{q}')$ and its possible *cluster property* are

$$\rho(\boldsymbol{q}, \boldsymbol{q}')$$

$$\stackrel{\text{def}}{=} \lim_n \frac{\int_{\Omega_n} \exp(-\beta U(\boldsymbol{q}, \boldsymbol{q}', \boldsymbol{q}_1, \ldots, \boldsymbol{q}_{N_n-2}))\, \mathrm{d}\boldsymbol{q}_1 \cdots \mathrm{d}\boldsymbol{q}_{N_n-2}}{(N_n - 2)! Z_0^c(\beta, \rho, V_n)}$$

$$\rho(\boldsymbol{q}, (\boldsymbol{q}' + \boldsymbol{\xi})) - \rho(\boldsymbol{q})\rho(\boldsymbol{q}' + \boldsymbol{\xi}) \underset{\xi \to \infty}{\longrightarrow} 0 \qquad [23]$$

where

$$Z_0^c \stackrel{\text{def}}{=} \int \mathrm{e}^{-\beta U(Q)} \mathrm{d}Q$$

is the "configurational" partition function.

The reader is referred to Ruelle (1969), Dobrushin (1968), Lanford and Ruelle (1969), and Gallavotti (1999).

Virial Theorem and Atomic Dimensions

For a long time it has been doubted that "just changing boundary conditions" could produce such dramatic changes as macroscopically different states (i.e., phase transitions in the sense of the definition in the last section). The first evidence that by taking the thermodynamic limit very regular analytic functions like $N^{-1} \log Z^c(\beta, N, V)$ (as a function of $\beta, v = V/N$) could develop, in the limit $\Omega \to \infty$, singularities like discontinuous derivatives (corresponding to the maximum in [16] being reached on a plateau and to a consequent existence of several pure phases) arose in the van der Waals' theory of liquid–gas transition.

Consider a real gas with N identical particles with mass m in a container Ω with volume V. Let the force acting on the ith particle be $\boldsymbol{f}_i$; multiplying both sides of the equations of motion, $m\ddot{\boldsymbol{q}}_i = \boldsymbol{f}_i$, by $-(1/2)\boldsymbol{q}_i$ and summing over i, it follows that

$$-\frac{1}{2}\sum_{i=1}^{N} m\boldsymbol{q}_i \cdot \ddot{\boldsymbol{q}}_i = -\frac{1}{2}\sum_{i=1}^{N} \boldsymbol{q}_i \cdot \boldsymbol{f}_i \stackrel{\text{def}}{=} \frac{1}{2} C(\boldsymbol{q})$$

and the quantity $C(\boldsymbol{q})$ defines the *virial of the forces* in the configuration $\boldsymbol{q}$. Note that $C(\boldsymbol{q})$ is not translation invariant because of the presence of the forces due to the walls.

Writing the force $\boldsymbol{f}_i$ as a sum of the internal and the external forces (due to the walls) the virial C can be expressed naturally as sum of the virial C_{int} of the internal forces (translation invariant) and of the virial C_{ext} of the external forces.

By dividing both sides of the definition of the virial by τ and integrating over the time interval $[0, \tau]$, one finds in the limit $\tau \to +\infty$, that is, up to quantities relatively infinitesimal as $\tau \to \infty$, that

$$\langle K \rangle = \tfrac{1}{2}\langle C \rangle \quad \text{and} \quad \langle C_{\text{ext}} \rangle = 3pV$$

where p is the pressure and V the volume. Hence

$$\langle K \rangle = \tfrac{3}{2} pV + \tfrac{1}{2}\langle C_{\text{int}} \rangle$$

or

$$\frac{1}{\beta} = pv + \frac{\langle C_{\text{int}} \rangle}{3N} \qquad [24]$$

Equation [24] is Clausius' *virial theorem*: in the case of no internal forces, it yields $\beta pv = 1$, the ideal-gas equation.

The internal virial C_{int} can be written, if $\boldsymbol{f}_{j \to i} = -\partial_{\boldsymbol{q}_i} \varphi(\boldsymbol{q}_i - \boldsymbol{q}_j)$, as

$$C_{\text{int}} = -\sum_{i=1}^{N} \sum_{i \neq j} \boldsymbol{f}_{j \to i} \cdot \boldsymbol{q}_i$$

$$\equiv -\sum_{i<j} \partial_{\boldsymbol{q}_i} \varphi(\boldsymbol{q}_i - \boldsymbol{q}_j) \cdot (\boldsymbol{q}_i - \boldsymbol{q}_j)$$

which shows that the contribution to the virial by the internal repulsive forces is negative while that of the attractive forces is positive. The average of C_{int} can be computed by the canonical distribution, which is convenient for the purpose. van der Waals first used the virial theorem to perform an actual computation of the corrections to the perfect-gas laws. Simply neglect the third-order term in the density and use the approximation $\rho(\boldsymbol{q}_1, \boldsymbol{q}_2) = \rho^2 \mathrm{e}^{-\beta\varphi(\boldsymbol{q}_1 - \boldsymbol{q}_2)}$ for the pair correlation function, [23], then

$$\frac{1}{2}\langle C_{\text{int}} \rangle = V \frac{3}{2\beta} \rho^2 I(\beta) + VO(\rho^3) \qquad [25]$$

where

$$I(\beta) = \frac{1}{2}\int (e^{-\beta\varphi(q)} - 1)d^3q$$

and the equation of state [24] becomes

$$pv + \frac{I(\beta)}{\beta v} + O(v^{-2}) = \beta^{-1}$$

For the purpose of illustration, the calculation of I can be performed approximately at "high temperature" (β small) in the case

$$\varphi(r) = 4\varepsilon\left(\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^{6}\right)$$

(the classical Lennard–Jones potential), $\varepsilon, r_0 > 0$. The result is

$$I \cong -(b - \beta a)$$

$$b = 4v_0,\ a = \frac{32}{3}\varepsilon v_0,\ v_0 = \frac{4\pi}{3}\left(\frac{r_0}{2}\right)^3$$

Hence,

$$pv + \frac{a}{v} - \frac{b}{\beta v} = \frac{1}{\beta} + O\left(\frac{1}{\beta v^2}\right)$$

$$\left(p + \frac{a}{v^2}\right)v = \left(1 + \frac{b}{v}\right)\frac{1}{\beta} = \frac{1}{1 - b/v}\,\frac{1}{\beta} + O\left(\frac{1}{\beta v^2}\right)$$

or

$$\left(p + \frac{a}{v^2}\right)(v - b)\beta = 1 + O(v^{-2}) \qquad [26]$$

which gives the equation of state for $\beta\varepsilon \ll 1$. Equation [26] can be compared with the well-known empirical *van der Waals equation* of state:

$$\beta\left(p + \frac{a}{v^2}\right)(v - b) = 1$$

or

$$(p + An^2/V^2)(V - nB) = nRT \qquad [27]$$

where, if N_A is Avogadro's number, $A = aN_A^2$, $B = bN_A, R = k_BN_A, n = N/N_A$. It shows the possibility of accessing the microscopic parameters ε and r_0 of the potential φ via measurements detecting deviations from the *Boyle–Mariotte law*, $\beta pv = 1$, of the rarefied gases: $\varepsilon = 3a/8b = 3A/8BN_A$ $r_0 = (3b/2\pi)^{1/3} = (3B/2\pi N_A)^{1/3}$.

As a final comment, it is worth stressing that the virial theorem gives in principle the exact corrections to the equation of state, in a rather direct and simple form, as time averages of the virial of the internal forces. Since the virial of the internal forces is easy to calculate from the positions of the particles as a function of time, the theorem provides a method for computing the equation of state in numerical simulations. In fact, this idea has been exploited in many numerical experiments, in which [24] plays a key role.

For more details, the reader is referred to Gallavotti (1999).

van der Waals Theory

Equation [27] is empirically used beyond its validity region (small density and small β) by regarding A, B as phenomenological parameters to be experimentally determined by measuring them near generic values of p, V, T. The measured values of A, B do not "usually vary too much" as functions of v, T and, apart from this small variability, the predictions of [27] have reasonably agreed with experience until, as experimental precision increased over the years, serious inadequacies eventually emerged.

Certain consequences of [27] are appealing: for example, **Figure 1** shows that it does not give a p monotonic nonincreasing in v if the temperature is small enough. A critical temperature can be defined as the largest value, T_c, of the temperature below which the graph of p as a function of v is not monotonic decreasing; the critical volume V_c is the value of v at the horizontal inflection point occurring for $T = T_c$.

For $T < T_c$ the van der Waals interpretation of the equation of state is that the function $p(v)$ may describe metastable states while the actual equilibrium states would follow an equation with a monotonic dependence on v and $p(v)$ becoming horizontal in the coexistence region of specific volumes. The precise value of p where to draw the plateau (see **Figure 1**) would then be fixed by experiment or theoretically predicted via the simple rule that the plateau associated with the represented isotherm is drawn at a height such that the area of the two cycles in the resulting loop are equal.

This is *Maxwell's rule*: obtained by assuming that the isotherm curve joining the extreme points of the plateau and the plateau itself define a cycle

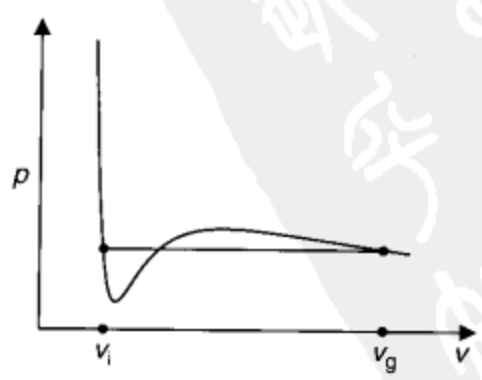

Figure 1 The van der Waals equation of state at a temperature $T < T_c$ where the pressure is not monotonic. The horizontal line illustrates the "Maxwell rule."

(see **Figure 1**) representing a sequence of possible macroscopic equilibrium states (the ones corresponding to the plateau) or states with extremely long time of stability ("metastable") represented by the curved part. This would be an isothermal Carnot cycle which, therefore, could not produce work: since the work produced in the cycle (i.e., $\oint p\mathrm{d}v$) is the signed area enclosed by the cycle the rule just means that the area is zero. The argument is doubtful at least because it is not clear that the intermediate states with p increasing with v could be realized experimentally or could even be theoretically possible.

A striking prediction of [27], taken literally, is that the gas undergoes a gas–liquid phase transition with a critical point at a temperature T_c, volume v_c, and pressure p_c that can be computed via [27] and are given by $RT_c = 8A/27B$, $V_c = 3B$ $(n = 1)$.

At the same time, the above prediction is interesting as it shows that there are simple relations between the critical parameters and the microscopic interaction constants, i.e., $\varepsilon \simeq k_B T_c$ and $r_0 \simeq (V_c/N_A))^{1/3}$: or more precisely $\varepsilon = 81k_B T_c/64$, $r_0 = (V_c/2\pi N_A)^{1/3}$ if a classical Lennard–Jones potential (i.e., $\varphi = 4\varepsilon((r_0/|q|)^{12} - (r_0/|q|)^6)$; see the last section) is used for the interaction potential φ.

However, [27] cannot be accepted acritically not only because of the approximations (essentially the neglecting of $O(v^{-1})$ in the equation of state), but mainly because, as remarked above, for $T < T_c$ the function p is no longer monotonic in v as it must be; see comment following [19].

The van der Waals equation, refined and complemented by Maxwell's rule, predicts the following behavior:

$$(p - p_c) \propto (v - v_c)^{\delta}, \quad \delta = 3, \ T = T_c$$
$$(v_g - v_l) \propto (T_c - T)^{\beta}, \quad \beta = 1/2, \quad \text{for } T \to T_c^- \qquad [28]$$

which are in sharp contrast with the experimental data gathered in the twentieth century. For the simplest substances, one finds instead $\delta \cong 5$, $\beta \cong 1/3$.

Finally, blind faith in the equation of state [27] is untenable, last but not least, also because nothing in the analysis would change if the space dimension was $d = 2$ or $d = 1$: but for $d = 1$, it is easily proved that the system, if the interaction decays rapidly at infinity, does not undergo phase transitions (see next section).

In fact, it is now understood that van der Waals' equation represents rigorously only a limiting situation, in which particles have a hard-core interaction (or a strongly repulsive one at close distance) and a further smooth interaction φ with very long range. More precisely, suppose that the part of the potential outside a hard-core radius $r_0 > 0$ is attractive (i.e., non-negative) and has the form $\gamma^d \varphi_1(\gamma^{-1}|q|) \leq 0$ and call $P_0(v)$ the (β-independent) product of β times the pressure of the hard-core system without any attractive tail ($P_0(v)$ is not explicitly known except if $d = 1$, in which case it is $P_0(v)(v - b) = 1, b = r_0$), and let

$$a = -\frac{1}{2}\int_{|q|>r_0} |\varphi_1(q)|\mathrm{d}q$$

If $p(\beta, v; \gamma)$ is the pressure when $\gamma > 0$ then it can be proved that

$$\beta p(\beta, v) \stackrel{\text{def}}{=} \lim_{\gamma \to 0} \beta p(\beta, v; \gamma) = \left[-\frac{\beta a}{v^2} + P_0(v)\right]_{\text{Maxwell's rule}} \qquad [29]$$

where the subscript means that the graph of $p(\beta, v)$ as a function of v is obtained from the function in square bracket by applying to it Maxwell's rule, described above in the case of the van der Waals equation. Equation [29] reduces exactly to the van der Waals equation for d = 1, and for d > 1 it leads to an equation with identical critical behavior (even though $P_0(v)$ cannot be explicitly computed).

The reader is referred to Lebowitz and Penrose (1979) and Gallavotti (1999) for more details.

Absence of Phase Transitions: $d = 1$

One of the most quoted no-go theorems in statistical mechanics is that one-dimensional systems of particles interacting via short-range forces do not exhibit phase transitions (cf. the next section) unless the somewhat unphysical situation of having zero absolute temperature is considered. This is particularly easy to check in the case of "nearest-neighbor hard-core interactions." Let the hard-core size be r_0, so that the interaction potential $\varphi(r) = +\infty$ if $r \leq r_0$, and suppose also that $\varphi(r) \equiv 0$ if $f \geq 2r_0$. In this case, the thermodynamic functions can be exactly computed and checked to be analytic: hence the equation of state cannot have any phase transition plateau. This is a special case of *van Hove's theorem* establishing smoothness of the equation of state for interactions extending beyond the nearest neighbor and rapidly decreasing at infinity.

If the definition of phase transition based on the sensitivity of the thermodynamic limit to variations of boundary conditions is adopted then a more general, conceptually simple, argument can be given to show that in one-dimensional systems there cannot be any phase transition if the potential energy of mutual interaction between a

configuration Q of particles to the left of a reference particle (located at the origin O, say) and a configuration Q' to the right of the particle (with $Q \cup O \cup Q'$ compatible with the hard cores) is uniformly bounded below. Then a mathematical proof can be devised showing that the influence of boundary conditions disappears as the boundaries recede to infinity. One also says that no long-range order can be established in a one-dimensional case, in the sense that one loses any trace of the boundary conditions imposed.

The analysis fails if the space dimension is ≥ 2: in this case, even if the interaction is short-ranged, the energy of interaction between two regions of space separated by a boundary is of the order of the boundary area. Hence, one cannot bound above and below the probability of any two configurations in two half-spaces by the product of the probabilities of the two configurations, each computed as if the other was not there. This is because such a bound would be proportional to the exponential of the surface of separation, which tends to ∞ when the surface grows large. This means that we cannot consider, at least not in general, the configurations in the two half-spaces as independently distributed.

Analytically, a condition on the potential sufficient to imply that the energy between a configuration to the left and one to the right of the origin is bounded below, if $d=1$, is simply expressed by

$$\int_{r'}^{\infty} r|\varphi(r)|\mathrm{d}r < +\infty \quad \text{for } r' > r_0$$

Therefore, in order to have phase transitions in $d=1$, a potential is needed that is "so long range" that it has a divergent first moment. It can be shown by counterexamples that if the latter condition fails there can be phase transitions even in $d=1$ systems.

The results just quoted also apply to discrete models like lattice gases or lattice spin models that will be considered later in the article.

For more details, we refer the reader to Landau and Lifschitz (1967), Dyson (1969), Gallavotti (1999), and Gallavotti *et al.* (2004).

Continuous Symmetries: "No $d=2$ Crystal" Theorem

A second case in which it is possible to rule out existence of phase transitions or at least of certain kinds of transitions arises when the system under analysis enjoys large symmetry. By symmetry is meant a group of transformations acting on the configurations and transforming each of them into a configuration which, at least for one boundary condition (e.g., periodic or open), has the same energy.

A symmetry is said to be "continuous" if the group of transformations is a continuous group. For instance, continuous systems have translational symmetry if considered in a container Ω with periodic boundary conditions. Systems with "too much symmetry" sometimes cannot show phase transitions. For instance, the continuous translation symmetry of a gas in a container Ω with periodic boundary conditions is sufficient to exclude the possibility of crystallization in dimension $d=2$.

To discuss this, which is a prototype of a proof which can be used to infer absence of many transitions in systems with continuous symmetries, consider the translational symmetry and a potential satisfying, besides the usual [14] and with the symbols used in [14], the further property that $|\boldsymbol{q}|^2|\partial_{ij}^2\varphi(\boldsymbol{q})| < \overline{B}|\boldsymbol{q}|^{-(d+\varepsilon_0)}$, with $\varepsilon_0 > 0$, for some $\overline{B}$ holds for $r_0 < |\boldsymbol{q}| \leq R$. This is a very mild extra requirement (and it allows for a hard-core interaction).

Consider an "ideal crystal" on a square lattice (for simplicity) of spacing a, exactly fitting in its container Ω of side L assumed with periodic boundary conditions: so that $N=(L/a)^d$ is the number of particles and a^{-d} is the density, which is supposed to be smaller than the close packing density if the interaction φ has a hard core. The probability distribution of the particles is rather trivial:

$$\overline{\mu} = \sum_{p} \prod_{n} \delta(\boldsymbol{q}_{p(n)} - a\,\boldsymbol{n}) \frac{\mathrm{d}\boldsymbol{Q}}{N!}$$

the sum running over the permutations $\boldsymbol{m} \to p(\boldsymbol{m})$ of the sites $\boldsymbol{m} \in \Omega, \boldsymbol{m} \in \mathbb{Z}^d, 0 < m_i \leq La^{-1}$. The density at $\boldsymbol{q}$ is

$$\widehat{\rho}(\boldsymbol{q}) = \sum_{\boldsymbol{n}} \delta(\boldsymbol{q} - a\,\boldsymbol{n}) \equiv \left\langle \sum_{j=1}^{N} \delta(\boldsymbol{q} - \boldsymbol{q}_j) \right\rangle$$

and its Fourier transform is proportional to

$$\rho(\boldsymbol{k}) \stackrel{\text{def}}{=} \frac{1}{N} \left\langle \sum_{j} \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{q}_j} \right\rangle, \quad \boldsymbol{k} = \frac{2\pi}{L}\boldsymbol{n}, \ \boldsymbol{n} \in \mathbb{Z}^d$$

$\rho(\boldsymbol{k})$ has value 1 for all $\boldsymbol{k}$ of the form $\boldsymbol{K}=(2\pi/a)\boldsymbol{n}$ and $(1/N)O(\max_{c=1,2}|\mathrm{e}^{ik_c a}-1|^{-2})$ otherwise. In presence of interaction, it has to be expected that, in a crystal state, $\rho(\boldsymbol{k})$ has peaks near the values $\boldsymbol{K}$: but the value of $\rho(\boldsymbol{k})$ can depend on the boundary conditions.

Since the system is translation invariant a crystal state defined as a state with a distribution "close" to $\overline{\mu}$,

i.e., with $\hat{\rho}(\boldsymbol{q})$ with peaks at the ideal lattice points $\boldsymbol{q}=\boldsymbol{na}$, cannot be realized under periodic boundary conditions, even when the system state is crystalline. To realize such a state, a symmetry-breaking term is needed in the interaction.

This can be done in several ways, for example, by changing the boundary condition. Such a choice implies a discussion of how much the boundary conditions influence the positions of the peaks of $\rho(\boldsymbol{k})$: for instance, it is not obvious that a boundary condition will not generate a state with a period different from the one that *a priori* has been selected for disproval (a possibility which would imply a reciprocal lattice of $\boldsymbol{K}$'s different from the one considered to begin with). Therefore, here the choice will be to imagine that an external weak force with potential $\varepsilon W(\boldsymbol{q})$ acts forcing a symmetry breaking that favors the occupation of regions around the points of the ideal lattice (which would mark the average positions of the particles in the crystal state that is being sought). The proof (*Mermin's theorem*) that no equilibrium state with particles distribution "close" to $\bar{\mu}$, i.e., with peaks in place of the delta functions (see below), is essentially reproduced below.

Take $W(\boldsymbol{q})=\sum_{\boldsymbol{na}\in\Omega}\chi(\boldsymbol{q}-\boldsymbol{na})$, where $\chi(\boldsymbol{q})\leq 0$ is smooth and zero everywhere except in a small vicinity of the lattice points around which it decreases to some negative minimum keeping a rotation symmetry around them. The potential W is invariant under translations by the lattice steps. By the choice of the boundary condition and εW, the density $\tilde{\rho}_\varepsilon(\boldsymbol{q})$ will be periodic with period a so that $\rho_\varepsilon(\boldsymbol{k})$ will, possibly, not have a vanishing limit as $N\to\infty$ only if $\boldsymbol{k}$ is a reciprocal vector $\boldsymbol{K}=(2\pi/a)\boldsymbol{n}$. If the potential is $\varphi+\varepsilon W$ and if there exists a crystal state in which particles have higher probability of being near the lattice points $\boldsymbol{na}$, it should be expected that for small $\varepsilon>0$ the system will be found in a state with Fourier transform of the density, $\rho_\varepsilon(\boldsymbol{k})$, satisfying, for some vector $\boldsymbol{K}\neq 0$ in the reciprocal lattice,

$$\lim_{\varepsilon\to 0}\lim_{N\to\infty}|\rho_\varepsilon(\boldsymbol{K})|=r>0 \qquad [30]$$

that is, the requirement is that uniformly in $\varepsilon\to 0$ the Fourier transform of the density has a peak at some $\boldsymbol{K}\neq\boldsymbol{0}$. Note that if $\boldsymbol{k}$ is not in the reciprocal lattice $\rho_\varepsilon(\boldsymbol{k})\underset{N\to\infty}{\longrightarrow}0$, being bounded above by

$$\frac{1}{N}O\left(\max_{j=1,2}|e^{ik_ja}-1|^{-2}\right)$$

because $(1/N)\tilde{\rho}_\varepsilon$ is periodic and its integral over $\boldsymbol{q}$ is equal to 1. Hence, excluding the existence of a crystal will be identified with the impossibility of the [30]. Other criteria can be imagined, for example, considering crystals with a lattice different from simple cubic, which lead to the same result by following the same technique. Nevertheless, it is not mathematically excluded (but unlikely) that, with some weaker existence definition, a crystal state could be possible even in two dimensions.

The following inequalities hold under the present assumptions on the potential and in the canonical distribution with periodic boundary conditions and parameters (β,ρ), $\rho=a^{-3}$ in a box Ω with side multiple of a (so that $N=(La^{-1})^d$) and potential of interaction $\varphi+\varepsilon W$. The further assumption that the lattice $\boldsymbol{na}$ is not a close-packed lattice is (of course) necessary when the interaction potential has a hard core. Then, for suitable $B_0,B,B_1,B_2>0$, independent of N, and ε and for $|\boldsymbol{\kappa}|<\pi/a$ and for all Ω (*if* $\boldsymbol{K}\neq\boldsymbol{0}$)

$$\frac{1}{N}\left\langle\left|\sum_{j=1}^{N}e^{-i(\boldsymbol{\kappa}+\boldsymbol{K})\cdot\boldsymbol{q}_j}\right|^2\right\rangle\geq B\frac{(\rho_\varepsilon(\boldsymbol{K})+\rho_\varepsilon(\boldsymbol{K}+2\boldsymbol{\kappa}))^2}{B_1\boldsymbol{\kappa}^2+\varepsilon B_2}$$

$$\frac{1}{N}\sum_{\boldsymbol{\kappa}}\gamma(\boldsymbol{\kappa})\frac{d\boldsymbol{\kappa}}{N}\left\langle\left|\sum_{j=1}^{N}e^{-i(\boldsymbol{\kappa}+\boldsymbol{K})\cdot\boldsymbol{q}_j}\right|^2\right\rangle\leq B_0<\infty \qquad [31]$$

where the averages are in the canonical distribution (β,ρ) with periodic boundary conditions and a symmetry-breaking potential $\varepsilon W(\boldsymbol{q})$; $\gamma(\boldsymbol{k})\geq 0$ is an (arbitrary) smooth function vanishing for $2|\boldsymbol{\kappa}|\geq\delta$ with $\delta<2\pi/a$ and B_0 depends on γ. See Appendix 3 for a derivation of [31].

Multiplying both sides of the first equation in [31] by $N^{-1}\gamma(\boldsymbol{\kappa})$ and summing over $\boldsymbol{\kappa}$, the crystallinity condition in the form [30] implies

$$B_0\geq Br^2a^d\int_{|\boldsymbol{\kappa}|<\delta}\frac{\gamma(\boldsymbol{\kappa})\,d\boldsymbol{\kappa}}{\boldsymbol{\kappa}^2B_1+\varepsilon B_2}$$

For $d=1,2$ the integral diverges, as $\varepsilon^{-1/2}$ or $\log\varepsilon^{-1}$, respectively, implying $|\rho_\varepsilon(\boldsymbol{K})|\underset{\varepsilon\to 0}{\longrightarrow}r=0$: the criterion of crystallinity, [30] cannot be satisfied if $d=1,2$.

The above inequality is an example of a general class of inequalities called *infrared inequalities* stemming from another inequality called *Bogoliubov's inequality* (see Appendix 3), which lead to the proof that certain kinds of ordered phases cannot exist if the dimension of the ambient space is $d=2$ when a finite volume, under suitable boundary conditions (e.g., periodic), shows a continuous symmetry. The excluded phenomenon is, more precisely, the nonexistence of equilibrium states exhibiting, in the thermodynamic limit, a symmetry lower than the continuous symmetry holding in a finite volume.

In general, existence of thermodynamic equilibrium states with symmetry lower than the

symmetry enjoyed by the system in finite volume and under suitable boundary conditions is called a "spontaneous symmetry breaking." It is yet another manifestation of instability with respect to changes in boundary conditions, hence its occurrence reveals a phase transition. There is a large class of systems for which an infrared inequality implies absence of spontaneous symmetry breaking: in most of the one- or two-dimensional systems a continuous symmetry cannot be spontaneously broken.

The limitation to dimension $d \leq 2$ is a strong limitation to the generality of the applicability of infrared theorems to exclude phase transitions. More precisely, systems can be divided into classes each of which has a "critical dimension" below which too much symmetry implies absence of phase transitions (or of certain kinds of phase transitions).

It should be stressed that, at the critical dimension, the symmetry breaking is usually so weakly forbidden that one might need astronomically large containers to destroy small effects (due to boundary conditions or to very small fields) which break the symmetry. For example, in the crystallization just discussed, the Fourier transform peaks are only bounded by $O(1/\sqrt{\log \varepsilon^{-1}})$. Hence, from a practical point of view, it might still be possible to have some kind of order even in large containers.

The reader is referred to Mermin (1968), Hohenberg (1969), and Ruelle (1969).

High Temperature and Small Density

There is another class of systems in which no phase transitions take place. These are the systems with stable and tempered interactions φ (e.g., those satisfying [14]) in the high-temperature and low-density region. The property is obtained by showing that the equation of state is analytic in the variables (β, ρ) near the origin $(0, 0)$.

A simple algorithm (*Mayer's series*) yields the coefficients of the virial series

$$\beta p(\beta, \rho) = \rho + \sum_{k=2}^{\infty} c_k(\beta) \rho^k$$

It has the drawback that the kth order coefficient $c_k(\beta)$ is expressed as a sum of many terms (a number growing more than exponentially fast in the order k) and it is not so easy (but possible) to show combinatorially that their sum is bounded exponentially in k if β is small enough. A more efficient approach leads quickly to the desired solution. Denoting $\mathbf{\Phi}(q_1, \ldots, q_n) \stackrel{\text{def}}{=} \sum_{i<j} \varphi(q_i - q_j)$, consider the ("spatial or configurational") correlation functions defined, in the grand canonical distribution with parameters β, λ (and empty boundary conditions), by

$$\rho_\Omega(q_1, \ldots, q_n) \stackrel{\text{def}}{=} \frac{1}{Z^{gc}(\beta, \lambda, V)} \sum_{m=0}^{\infty} z^{n+m} \times \int_\Omega \mathrm{e}^{-\beta \Phi(q_1, \ldots, q_n, y_1, \ldots, y_m)} \frac{\mathrm{d}y_1 \cdots \mathrm{d}y_m}{m!} \quad [32]$$

This is the probability density for finding particles with any momentum in the volume element $\mathrm{d}q_1 \cdots \mathrm{d}q_n$ (irrespective of where other particles are), and $z = \mathrm{e}^{\beta\lambda}(\sqrt{2\pi m \beta^{-1} h^{-2}})^d$ accounts for the integration over the momenta variables and is called the activity: it has the dimension of a density (cf. [23]).

Assuming that the potential has a hard core (for simplicity) of radius R, the interaction energy $\Phi_{q_1}(q_2, \ldots, q_n)$ of a particle at q_1 with any number of other particles at $q_2, \ldots, q_m$ with $|q_i - q_j| > R$ is bounded below by $-B$ for some $B \geq 0$ (related but not equal to the B in [14]). The functions ρ_Ω will be regarded as a sequence of functions "of one, two, ... particle positions": $\rho_\Omega = \{\rho_\Omega(q_1, \ldots, q_n)\}_{n=1}^{\infty}$ vanishing for $q_j \notin \Omega$. Then, one checks that

$$\rho_\Omega(q_1, \ldots, q_n) = z \delta_{n,1} \chi_\Omega(q_1) + K \rho_\Omega(q_1, \ldots, q_n) \quad [33a]$$

with

$$K\rho_\Omega(q_1, \ldots, q_n) \stackrel{\text{def}}{=} \mathrm{e}^{-\beta \Phi_{q_1}(q_2, \ldots, q_n)} (\rho_\Omega(q_2, \ldots, q_n) \delta_{n>1} + \sum_{s=1}^{\infty} \int_\Omega \frac{\mathrm{d}y_1 \cdots \mathrm{d}y_s}{s!} \prod_{k=1}^{s} (\mathrm{e}^{-\beta \varphi(q_1 - y_k)} - 1) \times \rho_\Omega(q_2, \ldots, q_n, y_1, \ldots, y_s)) \quad [33b]$$

where $\delta_{n,1}, \delta_{n>1}$ are Kronecker deltas and $\chi_\Omega(q)$ is the indicator function of Ω. Equation [33] is called the *Kirkwood–Salzburg equation* for the family of correlation functions in Ω. The kernel K of the equations is independent of Ω, but the domain of integration is Ω.

Calling α_Ω the sequence of functions $\alpha_\Omega(q_1, \ldots, q_n) \equiv 0$ if $n \neq 1$ and $\alpha_\Omega(q) = z\chi_\Omega(q)$, a recursive expansion arises, namely

$$\rho_\Omega = z\alpha_\Omega + z^2 K \alpha_\Omega + z^3 K^2 \alpha_\Omega + z^4 K^3 \alpha_\Omega + \cdots \quad [34]$$

It gives the correlation functions, provided the series converges. The inequality

$$|K^p \alpha_\Omega(q_1, \ldots, q_n)| \leq \mathrm{e}^{(2\beta B + 1)p} \left(\int |\mathrm{e}^{-\beta \varphi(q)} - 1| \mathrm{d}q \right)^p \stackrel{\text{def}}{=} \mathrm{e}^{(2\beta B + 1)p} r(\beta)^{3p} \quad [35]$$

shows that the series [34], called Mayer's series, converges if $|z| < \mathrm{e}^{-(2\beta B + 1)} r(\beta)^{-3}$. Convergence is uniform (as $\Omega \to \infty$) and $(K^p)\alpha_\Omega(q_1, \ldots, q_n)$ tends to a limit as $V \to \infty$ at fixed $q_1, \ldots, q_n$ and the limit is simply $(K^p \alpha)(q_1, \ldots, q_n)$, if $\alpha(q_1, \ldots, q_n) \equiv 0$ for $n \neq 1$, and $\alpha(q_1) \equiv 1$. This is because the kernel K contains

the factors $(e^{-\beta\varphi(q_1-y)}-1)$ which decay rapidly or, if φ has finite range, will eventually even vanish. It is also clear that $(K^p\alpha)(q_1,\ldots,q_n)$ is translation invariant.

Hence, if $|z|e^{2\beta B+1}r(\beta)^3<1$, the limits, as $\Omega\to\infty$, of the correlation functions exist and can be computed by a convergent power series in z; the correlation functions will be translation invariant (in the thermodynamic limit).

In particular, the one-point correlation function $\rho=\rho(q)$ is $\rho=z(1+O(zr(\beta)^3))$, which, to lowest order in z, just shows that activity and density essentially coincide when they are small enough. Furthermore, $\beta p_\Omega=(1/V)\log Z^{gc}(\beta,\lambda,V)$ is such that

$$z\partial_z\,\beta p_\Omega=\frac{1}{V}\int\rho_\Omega(q)\,dq$$

(from the definition of ρ_Ω in [32]). Therefore,

$$\begin{aligned}\beta p(\beta,z)&=\lim_{V\to\infty}\frac{1}{V}\log Z^{gc}(\beta,\lambda,V)\\&=\int_0^z\frac{dz'}{z'}\rho(\beta,z')\end{aligned}\qquad[36]$$

and, since the density ρ is analytic in z as well and $\rho\simeq z$ for z small, the grand canonical pressure is analytic in the density and $\beta p=\rho(1+O(\rho^2))$, at small density. In other words, the equation of state is, to lowest order, essentially the equation of a perfect gas. All quantities that are conceivably of some interest turn out to be analytic functions of temperature and density. The system is essentially a free gas and it has no phase transitions in the sense of a discontinuity or of a singularity in the dependence of a thermodynamic function in terms of others. Furthermore, the system cannot show phase transitions in the sense of sensitive dependence on boundary conditions of fixed external particles. This also follows, with some extra work, from the Kirkwood–Salzburg equations.

The reader is referred to Ruelle (1969) and Gallavotti (1969) for more details.

Lattice Models

The problem of proving the existence of phase transitions in models of homogeneous gases with pair interactions is still open. Therefore, it makes sense to study the problem of phase transitions in simpler models, tractable to some extent but nontrivial, and which are of practical interest in their own right.

The simplest models are the so-called lattice models in which particles are constrained to points of a lattice: they cannot move in the ordinary sense of the word (but, of course, they could jump) and therefore their configurations do not contain momentum variables.

The interaction energy is just the potential energy, and ensembles are defined as collections of probability distributions on the position coordinates of the particle configurations. Usually, the potential is a pair potential decaying fast at ∞ and, often, with a hard-core forbidding double or higher occupancy of the same lattice site. For instance, the *lattice gas* with potential φ, in a cubic box Ω with $|\Omega|=V=L^d$ sites of a square lattice with mesh $a>0$, is defined by the potential energy attributed to the configuration X of occupied distinct sites, i.e., subsets $X\subset\Omega$:

$$H(X)=-\sum_{(x,y)\in X}\varphi(x-y)\qquad[37]$$

where the sum is over pairs of distinct points in X. The canonical ensemble and the grand canonical ensemble are the collections of distributions, parametrized by $(\beta,\rho),(\rho=N/V)$, or, respectively, by (β,λ), attributing to X the probability

$$p_{\beta,\rho}(X)=\frac{e^{-\beta H(X)}}{Z_p^c(\beta,N,\Omega)}\delta_{|X|,N}\qquad[38a]$$

or

$$p_{\beta,\lambda}(X)=\frac{e^{\beta\lambda|X|}e^{-\beta H(X)}}{Z_p^{gc}(\beta,\lambda,\Omega)}\qquad[38b]$$

where the denominators are normalization factors that can, respectively, be called, in analogy with the theory of continuous systems, canonical and grand canonical partition functions; the subscript p stands for particles.

A lattice gas in which in each site there can be at most one particle can be regarded as a model for the distribution of a family of spins on a lattice. Such models are quite common and useful (e.g., they arise in studying systems with magnetic properties). Simply identify an "occupied" site with a "spin up" or $+$ and an "empty" site with a "spin down" or $-$ (say). If $\boldsymbol{\sigma}=\{\sigma_x\}_{x\in\Omega}$ is a spin configuration, the energy of the configuration "for potential φ and magnetic field h" will be

$$H(\boldsymbol{\sigma})=-\sum_{(x,y)\in\Omega}\varphi(x-y)\sigma_x\sigma_y-h\sum_x\sigma_x\qquad[39]$$

with the sum running over pairs $(x,y)\in\Omega$ of distinct sites. If $\varphi(x-y)\equiv J_{xy}\geq 0$, the model is called a *ferromagnetic Ising model*. As in the case of continuous systems, it will be assumed to have a finite range for φ: that is, $\varphi(x)=0$ for $|x|>R$, for some R, unless explicitly stated otherwise.

The canonical and grand canonical ensembles in the box Ω with respective parameters (β, m) or (β, h) will be defined as the probability distributions on the spin configurations $\boldsymbol{\sigma} = \{\sigma_x\}_{x\in\Omega}$ with $\sum_{x\in\Omega}\sigma_x = M = mV$ or without constraint on M, respectively; hence,

$$p_{\beta,m}(\boldsymbol{\sigma}) = \frac{\exp\left(-\beta\sum_{(x,y)}\varphi(x-y)\sigma_x\sigma_y\right)}{Z_s^c(\beta, M, \Omega)}$$

$$p_{\beta,h}(\boldsymbol{\sigma}) = \frac{\exp\left(-\beta h\sum\sigma_x - \beta\sum_{(x,y)}\varphi(x-y)\sigma_x\sigma_y\right)}{Z_s^{gc}(\beta, h, \Omega)} \qquad [40]$$

where the denominators are normalization factors again called, respectively, the canonical and grand canonical partition functions. As in the study of the previous continuous systems, canonical and grand canonical ensembles with "external fixed particle configurations" can be defined together with the corresponding ensembles with "external fixed spin configurations"; the subscript s stands for spins.

For each configuration $X \subset \Omega$ of a lattice gas, let $\{n_x\}$ be $n_x = 1$ if $x \in X$ and $n_x = 0$ if $x \notin X$. Then the transformation $\sigma_x = 2n_x - 1$ establishes a correspondence between lattice gas and spin distributions. In the correspondence, the potential $\varphi(x-y)$ of the lattice gas generates a potential $(1/4)\varphi(x-y)$ for the corresponding spin system and the chemical potential λ for the lattice gas is associated with a magnetic field h for the spin system with $h = (1/2)(\lambda + \sum_{x\neq 0}\varphi(x))$.

The correspondence between boundary conditions is natural: for instance, a boundary condition for the lattice gas in which all external sites are occupied becomes a boundary condition in which external sites contain a spin $+$. The close relation between lattice gas and spin systems permits switching from one to the other with little discussion.

In the case of spin systems, empty boundary conditions are often considered (no spins outside Ω). In lattice gases and spin systems (as well as in continuum systems), often periodic and semiperiodic boundary conditions are considered (i.e., periodic in one or more directions and with empty or fixed external particles or spins in the others).

Thermodynamic limits for the partition functions

$$\begin{aligned}
-\beta f(\beta, v) &= \lim_{\substack{\Omega\to\infty \\ V/N\to v}} \frac{1}{N}\log Z_p^c(\beta, N, \Omega) \\
\beta p(\beta, \lambda) &= \lim_{\Omega\to\infty} \frac{1}{V}\log Z_p^{gc}(\beta, \lambda, \Omega) \\
-\beta g(\beta, m) &= \lim_{\substack{\Omega\to\infty, \\ M/V\to m}} \frac{1}{V}\log Z_s^c(\beta, M, \Omega) \\
\beta f(\beta, h) &= \lim_{\Omega\to\infty} \frac{1}{V}\log Z_s^{gc}(\beta, \lambda, \Omega)
\end{aligned} \qquad [41]$$

can be shown to exist by a method similar to the one discussed in Appendix 2. They have convexity and continuity properties as in the cases of the continuum systems. In the case of a lattice gas, the f, p functions are still interpreted as free energy and pressure, respectively. In the case of spin, $f(\beta, h)$ has the interpretation of magnetic free energy, while $g(\beta, m)$ does not have a special name in the thermodynamics of magnetic systems. As in the continuum systems, it is occasionally useful to define infinite-volume equilibrium states:

Definition An infinite-volume state with parameters (β, h) or (β, m) is a collection of average values $F \to \langle F\rangle$ obtained, respectively, as limits of finite-volume averages $\langle F\rangle_{\Omega_n}$ defined from canonical or grand canonical distributions in Ω_n with fixed parameters (β, h) or (β, m), or (u, v) and with general boundary condition of fixed external spins or empty sites, on sequences $\Omega_n \to \infty$ for which such limits exist simultaneously for all local observables F.

This is taken verbatim from the definition in the section "Phase transitions and boundary conditions." In this way, it makes sense to define the spin correlation functions for $X = (\xi_1, \ldots, \xi_n)$ as $\langle\sigma_X\rangle$ if $\sigma_X = \prod_j \sigma_{\xi_j}$. For instance, we shall call $\rho(\xi_1, \xi_2) \stackrel{\text{def}}{=} \langle\sigma_{\xi_1}\sigma_{\xi_2}\rangle$ and a pure phase can be defined as an infinite-volume state such that

$$\langle\sigma_X\sigma_{Y+\xi}\rangle - \langle\sigma_X\rangle\langle\sigma_{Y+\xi}\rangle \underset{\xi\to\infty}{\longrightarrow} 0 \qquad [42]$$

Again, for more details, we refer the reader to Ruelle (1969) and Gallavotti (1969).

Thermodynamic Limits and Inequalities

An interesting property of lattice systems is that it is possible to study delicate questions like the existence of infinite-volume states in some (moderate) generality. A typical tool is the use of inequalities. As the simplest example of a vast class of inequalities, consider the ferromagnetic Ising model with some finite (but arbitrary) range interaction $J_{xy} \geq 0$ in a field $h_x \geq 0$: J, h may even be not translationally invariant. Then the average of $\sigma_X \stackrel{\text{def}}{=} \sigma_{x_1}\sigma_{x_2}\cdots\sigma_{x_n}$, $X = (x_1, \ldots, x_n)$, in a state with "empty boundary conditions" (i.e., no external spins) satisfies the inequalities

$$\langle\sigma_X\rangle,\ \partial_{h_x}\langle\sigma_X\rangle,\ \partial J_{xy}\langle\sigma_X\rangle \geq 0 \quad X = (x_1, \ldots, x_n)$$

More generally, let $H(\boldsymbol{\sigma})$ in [39] be replaced by $H(\boldsymbol{\sigma}) = -\sum_X J_X\sigma_X$ with $J_X \geq 0$ and X can be any finite set; then, if $Y = (y_1, \ldots, y_n)$, $X = (x_1, \ldots, x_n)$, the following *Griffiths inequalities* hold:

$$\langle\sigma_X\rangle \geq 0, \quad \partial_{J_Y}\langle\sigma_X\rangle \equiv \langle\sigma_X\sigma_Y\rangle - \langle\sigma_X\rangle\langle\sigma_Y\rangle \geq 0 \qquad [43]$$

The inequalities can be used to check, in ferromagnetic Ising models, [39], existence of infinite-volume states (cf. the sections "Phase transitions and boundary conditions" and "Lattice models") obtained by fixing the boundary condition $\mathcal{B}$ to be either "all external spins $+$" or "all external sites empty." If $\langle F\rangle_{\mathcal{B},\Omega}$ denotes the grand canonical average with boundary condition $\mathcal{B}$ and any fixed $\beta, h > 0$, this means that for all local observables $F(\sigma_\Lambda)$ (i.e., for all F depending on the spin configuration in any fixed region Λ) all the following limits exist:

$$\lim_{\Omega\to\infty} \langle F\rangle_{\mathcal{B},\Omega} = \langle F\rangle_{\mathcal{B}} \qquad [44]$$

The reason is that the inequalities [43] imply that all averages $\langle\sigma_X\rangle_{\mathcal{B},\Omega}$ are monotonic in Ω for all fixed $X \subset \Omega$: so the limit [44] exists for $F(\sigma) = \sigma_X$. Hence, it exists for all F's depending only on finitely many spins, because any local function F "measurable in Λ" can be expressed (uniquely) as a linear combination of functions σ_X with $X \subseteq \Lambda$.

Monotonicity with empty boundary conditions is seen by considering the sites outside Ω and in a region Ω' with side one unit larger than that of Ω and imagining that the couplings J_X with $X \subset \Omega'$ but $X \not\subset \Omega$ vanish. Then, $\langle\sigma_X\rangle_{\Omega'} \geq \langle\sigma_X\rangle_{\Omega}$, because $\langle\sigma_X\rangle_{\Omega'}$ is an average computed with a distribution corresponding to an energy with the couplings J_X with $X \not\subset \Omega$, but $X \subset \Omega'$, changed from 0 to $J_X \geq 0$.

Likewise, if the boundary condition is $+$, then enlarging the box from Ω to Ω' corresponds to decreasing an external field h acting on the external spins from $+\infty$ (which would force all external spins to be $+$) to a finite value $h \geq 0$: so, increasing the box Ω causes $\langle\sigma_X\rangle_{+,\Omega}$ to decrease. Therefore, as Ω increases, Ising ferromagnets spin correlations increase if the boundary condition is empty and decrease if it is $+$.

The inequalities can be used in similar ways to prove that the infinite-volume states obtained from $+$ or empty boundary conditions are translation invariant; and that in zero external field, $h = 0$, the $+$ and $-$ boundary conditions generate pure states if the interaction potential is only a pair ferromagnetic interaction.

There are many other important inequalities which can be used to prove several existence theorems along very simple paths. Unfortunately, their use is mostly restricted to lattice systems and requires very special assumptions on the energy (e.g., ferromagnetic interactions in the above example). The quoted examples were among the first discovered and provide a way to exhibit nontrivial thermodynamic limits and pure states.

For more details, see Ruelle (1969), Lebowitz (1974), Gallavotti (1999), Lieb and Thirring (2001), and Lieb (2002).

Symmetry-Breaking Phase Transitions

The simplest phase transitions (see the section "Phase transitions and boundary conditions") are symmetry-breaking transitions in lattice systems: they take place when the energy of the system in a container Ω and with some special boundary condition (e.g., periodic, antiperiodic, or empty) is invariant with respect to the action of a group $\mathcal{G}$ on phase space. This means that on the points x of phase space acts a group of transformations $\mathcal{G}$ so that with each $\gamma \in \mathcal{G}$ is associated a map $x \to x\gamma$ which transforms x into $x\gamma$ respecting the composition law in $\mathcal{G}$, that is, $(x\gamma)\gamma' \equiv x(\gamma\gamma')$. If F is an observable, the action of the group on phase space induces an action on the observable F changing $F(x)$ into $F_\gamma(x) \stackrel{\text{def}}{=} F(x\gamma^{-1})$.

A symmetry-breaking transition occurs when, by fixing suitable boundary conditions and taking the thermodynamic limit, a state $F \to \langle F\rangle$ is obtained in which some local observable shows a nonsymmetric average $\langle F\rangle \neq \langle F_\gamma\rangle$ for some γ.

An example is provided by the "nearest-neighbor ferromagnetic Ising model" on a d-dimensional lattice with energy function given by [39] with $h = 0$ and $\varphi(x-y) \equiv 0$ unless $|x-y| = 1$, i.e., unless x, y are nearest neighbors, in which case $\varphi(x-y) = J > 0$. With periodic or empty boundary conditions, it exhibits a discrete "up–down" symmetry $\sigma \to -\sigma$.

Instability with respect to boundary conditions can be revealed by considering the two boundary conditions, denoted $+$ or $-$, in which the lattice sites outside the container Ω are either occupied by spins $+$ or by spins $-$. Consider also, for later reference, (1) the boundary conditions in which the boundary spins in the upper half of the boundary are $+$ and the ones in the lower part are $-$: call this the $\pm$-boundary condition (see **Figure 2**); or (2) the boundary conditions in

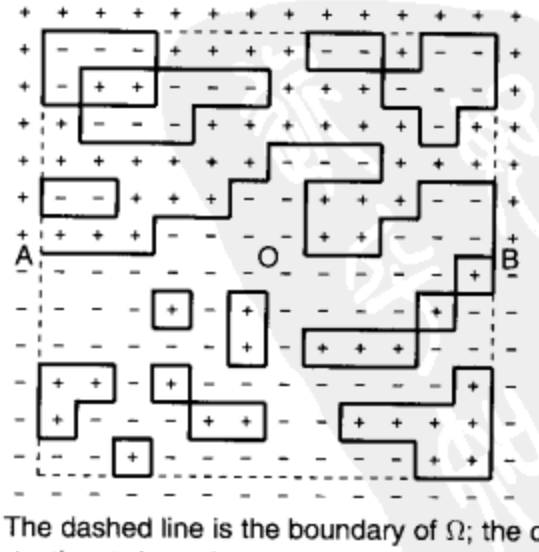

Figure 2 The dashed line is the boundary of Ω; the outer spins correspond to the $\pm$ boundary condition. The points *A*, *B* are points where an open "line" λ ends.

which some of the opposite sides of Ω are identified while + or − conditions are assigned on the remaining sides: call these "cylindrical or semiperiodic boundary conditions."

A new description of the spin configurations is useful: given $\boldsymbol{\sigma}$, draw a unit segment perpendicular to the center of each bond b having opposite spins at its extremes. An example of this construction is provided by **Figure 2** for the boundary condition ±.

The set of segments can be grouped into lines separating regions where the spins are positive from regions where they are negative. If the boundary condition is + or −, the lines form "closed polygons", whereas, if the condition is ±, there is also a single polygon λ_1 which is not closed (as in **Figure 2**). If the boundary condition is periodic or cylindrical, all polygons are closed but some may "go around" Ω. The polygons are also called "contours" and the length of a polygon γ will be denoted $|\gamma|$.

The correspondence $(\gamma_1, \gamma_2, \ldots, \gamma_n, \lambda_1) \longleftrightarrow \boldsymbol{\sigma}$, for the boundary condition ± or, for the boundary condition + (or −), $\boldsymbol{\sigma} \longleftrightarrow (\gamma_1, \ldots, \gamma_n)$ is one-to-one and, if $h = 0$, the energy $H_\Omega(\boldsymbol{\sigma})$ of a configuration is higher than $-J \times$(number of bonds in Ω) by an amount $2J(|\lambda_1| + \sum_i |\gamma_i|)$ or, respectively, $2J \sum_i |\gamma_i|$. The grand canonical probability of each spin configuration is therefore proportional, if $h = 0$, respectively, to

$$e^{-2\beta J(|\lambda_1| + \sum_i |\gamma_i|)} \quad \text{or} \quad e^{-2\beta J \sum_i |\gamma_i|} \qquad [45]$$

and the "up–down" symmetry is clearly reflected by [45].

The average $\langle \sigma_x \rangle_{\Omega,+}$ of σ_+ with + boundary conditions is given by $\langle \sigma_x \rangle_{\Omega,+} = 1 - 2P_{\Omega,+}(-)$, where $P_{\Omega,+}(-)$ is the probability that the spin σ_x is –1. If the site x is occupied by a negative spin then the point x is inside some contour γ associated with the spin configuration $\boldsymbol{\sigma}$ under consideration. Hence, if $\rho(\gamma)$ is the probability that a given contour belongs to the set of contours describing a configuration $\boldsymbol{\sigma}$, it is $P_{\Omega,+}(-) \leq \sum_{\gamma o x} \rho(\gamma)$ where $\gamma o x$ means that γ "surrounds" x.

If $\Gamma = (\gamma_1, \ldots, \gamma_n)$ is a spin configuration and if the symbol $\Gamma \mathrm{comp} \gamma$ means that the contour γ is "disjoint" from $\gamma_1, \ldots, \gamma_n$ (i.e., $\{\gamma \cup \Gamma\}$ is a new spin configuration), then

$$\begin{aligned} \rho(\gamma) &= \frac{\sum_{\Gamma \ni \gamma} e^{-2\beta J \sum_{\gamma' \in \Gamma} |\gamma'|}}{\sum_{\Gamma} e^{-2\beta J \sum_{\gamma' \in \Gamma} |\gamma'|}} \\ &\equiv e^{-2\beta J|\gamma|} \frac{\sum_{\Gamma \mathrm{comp} \gamma} e^{-2\beta J \sum_{\gamma' \in \Gamma} |\gamma'|}}{\sum_{\Gamma} e^{-2\beta J \sum_{\gamma' \in \Gamma} |\gamma'|}} \\ &\leq e^{-2\beta J|\gamma|} \end{aligned} \qquad [46]$$

because the last ratio in [46] does not exceed 1. Note that there are $> 3^p$ different shapes of γ with perimeter p and at most p^2 congruent γ's containing x; therefore, the probability that the spin at x is − when the boundary condition is + satisfies the inequality

$$P_{\Omega,+}(-) \leq \sum_{p=4}^{\infty} p^2 3^p e^{-2\beta J p} \underset{\beta \to \infty}{\longrightarrow} 0$$

This probability can be made arbitrarily small so that $\langle \sigma_x \rangle_{\Omega,+}$ is estimated by a quantity which is as close to 1 as desired provided β is large enough and the closeness of $\langle \sigma_x \rangle_{\Omega,+}$ to 1 is estimated by a quantity which is both x and Ω independent.

A similar argument for the (−)-boundary condition, or the remark that for $h = 0$ it is $\langle \sigma_x \rangle_{\Omega,-} = -\langle \sigma_x \rangle_{\Omega,+}$, leads to conclude that, at large β, $\langle \sigma_x \rangle_{\Omega,-} \neq \langle \sigma_x \rangle_{\Omega,+}$ and the difference between the two quantities is positive uniformly in Ω. This is the proof (*Peierls' theorem*) of the fact that there is, if β is large, a strong instability, of the magnetization with respect to the boundary conditions, i.e., the nearest-neighbor Ising model in dimension 2 (or greater, by an identical argument) has a phase transition. If the dimension is 1, the argument clearly fails and no phase transition occurs (see the section "Absence of phase transitions: $d = 1$").

For more details, see Gallavotti (1999).

Finite-Volume Effects

The description in the last section of the phase transition in the nearest-neighbor Ising model can be made more precise both from physical and mathematical points of view giving insights into the nature of the phase transitions. Assume that the boundary condition is the (+)-boundary condition and describe a spin configuration $\boldsymbol{\sigma}$ by means of the associated closed disjoint polygons $(\gamma_1, \ldots, \gamma_n)$. Attribute to $\boldsymbol{\sigma} = (\gamma_1, \ldots, \gamma_n)$ a probability proportional to [45]. Then the following *Minlos–Sinai's theorem* holds:

Theorem *If β is large enough there exist $C > 0$, $\rho(\gamma) > 0$ with $\rho(\gamma) \leq e^{-2\beta J|\gamma|}$ and such that a spin configuration $\boldsymbol{\sigma}$ randomly chosen out of the grand canonical distribution with + boundary conditions and $h = 0$ will contain, with probability approaching 1 as $\Omega \to \infty$, a number $K_{(\gamma)}(\boldsymbol{\sigma})$ of contours congruent to γ such that*

$$|K_{(\gamma)}(\boldsymbol{\sigma}) - \rho(\gamma)|\Omega|| \leq C\sqrt{|\Omega|}\, e^{-\beta J|\gamma|} \qquad [47]$$

and this relation holds simultaneously for all γ's.

Thus, there are very few contours (and the larger they are the smaller is, in absolute and relative value, their number): a typical spin configuration in the grand canonical ensemble with (+)-boundary conditions is such that the large majority of the spins is "positive" and, in the "sea" of positive spins, there are a few negative spins distributed in small and rare regions (their number, however, is still of order of $|\Omega|$).

Another consequence of the analysis in the last section concerns the the approximate equation of state near the phase transition region at low temperatures and finite Ω. If Ω is finite, the graph of h versus $m_\Omega(\beta, h)$ will have a rather different behavior depending on the possible boundary conditions. For example, if the boundary condition is $(+)$ or $(-)$, one gets, respectively, the results depicted in **Figure 3a** and **3b**, where $m^*(\beta)$ denotes the spontaneous magnetization (i.e., $m^*(\beta) \stackrel{\text{def}}{=} \lim_{h\to 0^+} \lim_{\Omega\to\infty} m_\Omega(\beta, h)$).

With periodic or empty boundary conditions, the diagram changes as in **Figure 4**. The thermodynamic limit $m(\beta, h) = \lim_{\Omega\to\infty} m_\Omega(\beta, h)$ exists for all $h \neq 0$ and the resulting graph is in **Figure 4b**, which shows that at $h = 0$ the limit is discontinuous. It can be proved, if β is large enough, that $\infty > \lim_{h\to 0^+} \partial_h m(\beta, h) = \chi(\beta) > 0$ (i.e., the angle between the vertical part of the graph and the rest is sharp).

Furthermore, it can be proved that $m(\beta, h)$ is analytic in h for $h \neq 0$. If β is small enough, analyticity holds at all h. For β large, the function $f(\beta, h)$ has an essential singularity at $h = 0$: a result that can be interpreted as excluding a naive theory of metastability as a description of states governed by an equation of state obtained from an analytic continuation to negative values of h of $f(\beta, h)$.

The above considerations and results further clarify the meaning of a phase transition for a finite system. For more details, we refer the reader to Gallavotti (1999) and Friedli and Pfister (2004).

Beyond Low Temperatures (Ferromagnetic Ising Model)

A limitation of the results discussed above is the condition of low temperature ("β large enough"). A natural problem is to go beyond the low-temperature region and to describe fully the phenomena in the region where boundary condition instability takes place and first develops. A number of interesting partial results are known, which considerably improve the picture emerging from the previous analysis. A striking list, but far from exhaustive, of such results follows and focuses on the properties of ferromagnetic Ising spin systems. The reason for restricting to such cases is that they are simple enough to allow a rather fine analysis, which sheds considerable light on the structure of statistical mechanics suggesting precise formulation

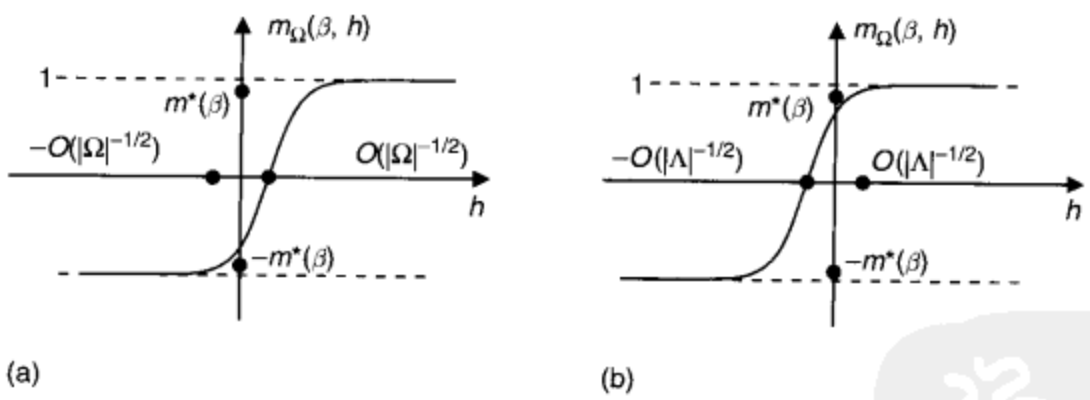

Figure 3 The h vs $m_\Omega(\beta, h)$ graphs for Ω finite and (a) $+$ and (b) $-$ conditions.

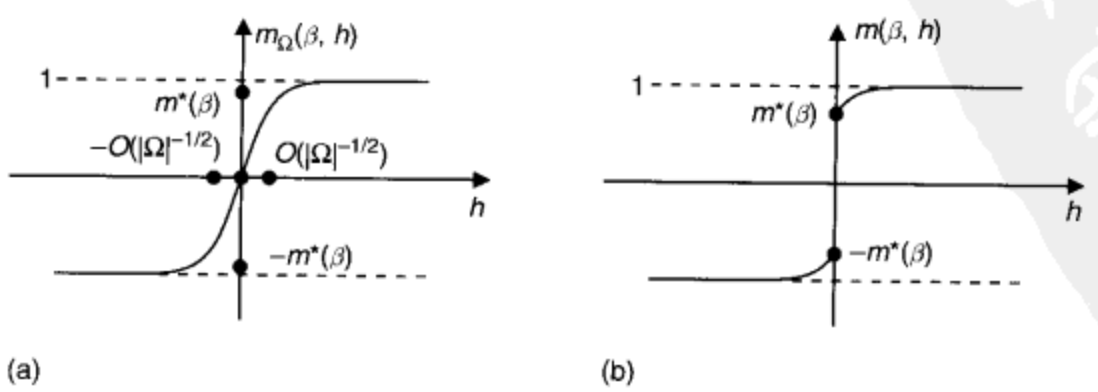

Figure 4 (a) The h vs $m_\Omega(\beta, h)$ graph for periodic or empty boundary conditions. (b) The discontinuity (at $h = 0$) of the thermodynamic limit.

of the problems that it would be desirable to understand in more general systems.

1. Let $z \stackrel{\text{def}}{=} e^{\beta h}$ and consider that the product of z^V (V is the number of sites $|\Omega|$ of Ω) times the partition function with periodic or perfect-wall boundary conditions and with finite-range ferromagnetic interaction, not necessarily nearest-neighbor; a polynomial in z (of degree $2V$) is thus obtained. Its zeros lie on the unit circle $|z|=1$: this is *Lee–Yang's theorem*. It implies that the only singularities of $f(\beta, h)$ in the region $0 < \beta < \infty, -\infty < h < +\infty$ can be found at $h=0$.

   A singularity can appear only if the point $z=1$ is an accumulation point of the limiting distribution (as $\Omega \to \infty$) of the zeros on the unit circle: if the zeros are $z_1, \ldots, z_{2V}$ then

$$\frac{1}{V}\log z^V Z(\beta, h, \Omega, \text{periodic}) = 2\beta J + \beta h + \frac{1}{V}\sum_{i=1}^{2V}\log(z - z_i)$$

   and if

$$V^{-1} \times (\text{number of zeros of the form } z_j = e^{i\theta_j}, \theta \le \theta_j \le \theta + d\theta) \underset{\Omega\to\infty}{\longrightarrow} \frac{d\rho_\beta(\theta)}{2\pi}$$

   it is

$$\beta f(\beta, h) = 2\beta J + \frac{1}{2\pi}\int_{-\pi}^{\pi}\log(z - e^{i\theta})\, d\rho_\beta(\theta) \qquad [48]$$

   The existence of the measure $d\rho_\beta(\theta)$ follows from the existence of the thermodynamic limit: but $d\rho_\beta(\theta)$ is not necessarily $d\theta$-continuous, i.e., not necessarily proportional to $d\theta$.
2. It can be shown that, with not necessarily a nearest-neighbor interaction, the zeros of the partition function do not move too much under small perturbations of the potential even if one perturbs the energy (at perfect-wall or periodic boundary conditions) into

$$H'_\Omega(\boldsymbol{\sigma}) = H_\Omega(\boldsymbol{\sigma}) + (\delta H_\Omega)(\boldsymbol{\sigma})$$
$$(\delta H_\Omega)(\boldsymbol{\sigma}) = \sum_{X\subset\Omega} J'(X)\,\sigma_X \qquad [49]$$

   where $J'(X)$ is very general and defined on subsets $X = (x_1, \ldots, x_k) \subset \Omega$ such that the quantity $||J'|| = \sup_{y\in Z^d}\sum_{y\in X}|J'(X)|$ is small enough. More precisely, with a ferromagnetic pair potential J fixed, suppose that one knows that, when $J'=0$, the partition function zeros in the variable $z = e^{\beta h}$ lie in a certain closed set N (of the unit circle) in the z-plane. Then, if $J' \neq 0$, they lie in a closed set N^1, Ω-independent and contained in a neighborhood of N of width shrinking to 0 when $||J'|| \to 0$. This allows to establish various relations between analyticity properties and boundary condition instability as described in (3) below.
3. In the ferromagnetic Ising model, with not necessarily a nearest-neighbor interaction, one says that there is a gap around 0 if $d\rho_\beta(\theta) = 0$ near $\theta = 0$. It can be shown that if β is small enough there is a gap for all h of width *uniform* in h.
4. Another question is whether the boundary condition instability is always revealed by the one-spin correlation function (i.e., by the magnetization) or whether it might be shown only by some correlation functions of higher order. It can be proved that no boundary condition instability occurs for $h \neq 0$; at $h=0$ it is possible only if

$$\lim_{h\to 0^-} m(\beta, h) \neq \lim_{h\to 0^+} m(\beta, h) \qquad [50]$$

5. A consequence of the Griffiths' inequalities (cf. the section "Thermodynamic limits and inequalities") is that if [50] is true for a given β_0 then it is true for all $\beta > \beta_0$. Therefore, item (4) leads to a natural definition of the critical temperature T_c as the least upper bound of the T's such that [50] holds ($k_B T = \beta^{-1}$).
6. If $d=2$ the free energy of the nearest-neighbor ferromagnetic Ising model has a singularity at β_c and the value of β_c is known exactly from the exact solutions of the model: $m(\beta, 0^+) \stackrel{\text{def}}{=} m^*(\beta) \equiv (1 - \sinh^4 2\beta J)^{1/8}$. The location and nature of the singularities of $f(\beta, 0)$ as a function of β remains an open question for $d=3$. In particular, the question whether there is a singularity of $f(\beta, 0)$ at $\beta = \beta_c$ is open.
7. For $\beta < \beta_c$ there is instability with respect to boundary conditions (see (6) above) and a natural question is: how many "pure" phases can exist in the ferromagnetic Ising model? (cf. the section "Phase transitions and boundary conditions," eqn [22]). Intuition suggests that there should be only two phases: the positively magnetized and the negatively magnetized ones.

   One has to distinguish between translation-invariant pure phases and non-translation-invariant ones. It can be proved that, in the case of the two-dimensional nearest-neighbor ferromagnetic Ising models, all infinite-volume states (cf. the section "Lattice models") are translationally invariant. Furthermore, they can be obtained by

considering just the two boundary conditions + and −: the latter states are also pure states for models with non-nearest-neighbor ferromagnetic interaction. The solution of this problem has led to the introduction of many new ideas and techniques in statistical mechanics and probability theory.

8. In any dimension $d \geq 2$, for β large enough, it can be proved that the nearest-neighbor Ising model has only two translation-invariant phases. If the dimension is ≥ 3 and β is large, the + and − phases exhaust the set of translation-invariant pure phases but there exist non-translation-invariant phases. For β close to β_c, however, the question is much more difficult.

For more details, see Onsager (1944), Lee and Yang (1952), Ruelle (1971), Sinai (1991), Gallavotti (1999), Aizenman (1980), Higuchi (1981), and Friedli and Pfister (2004).

Geometry of Phase Coexistence

Intuition about the phenomena connected with the classical phase transitions is usually based on the properties of the liquid–gas phase transition; this transition is usually experimentally investigated in situations in which the total number of particles is fixed (canonical ensemble) and in presence of an external field (gravity).

The importance of such experimental conditions is obvious; the external field produces a nontranslationally invariant situation and the corresponding separation of the two phases. The fact that the number of particles is fixed determines, on the other hand, the fraction of volume occupied by each of the two phases.

Once more, consider the nearest-neighbor ferromagnetic Ising model: the results available for it can be used to obtain a clear picture of the solution to problems that one would like to solve but which in most other models are intractable with present-day techniques.

It will be convenient to discuss phase coexistence in the canonical ensemble distributions on configurations of fixed total magnetization $M = mV$ (see the section "Lattice models"; [40]). Let β be large enough to be in the two-phase region and, for a fixed $\alpha \in (0, 1)$, let

$$\begin{aligned} m &= \alpha\, m^*(\beta) + (1-\alpha)\,(-m^*(\beta)) \\ &= (1-2\alpha)\, m^*(\beta) \end{aligned} \qquad [51]$$

that is, m is in the vertical part of the diagram $m = m(\beta, h)$ at β fixed (see **Figure 4**).

Fixing m as in [51] does not yet determine the separation of the phases in two different regions; for this effect, it will be necessary to introduce some external cause favoring the occupation of a part of the volume by a single phase. Such an asymmetry can be obtained in at least two ways: through a weak uniform external field (in complete analogy with the gravitational field in the liquid–vapor transition) or through an asymmetric field acting only on boundary spins. The latter should have the same qualitative effect as the former, because in a phase transition region a boundary perturbation produces volume effects (see sections "Phase transitions and inequalities" and "Symmetry-breaking phase transitions"). From a mathematical point of view, it is simpler to use a boundary asymmetry to produce phase separations and the simplest geometry is obtained by considering $\pm$-cylindrical or $++$-cylindrical boundary conditions: this means $++$ or $\pm$ boundary conditions periodic in one direction (e.g., in **Figure 2** imagine the right and left boundary identified after removing the boundary spins on them).

Spins adjacent to the bases of Ω act as symmetry-breaking external fields. The $++$-cylindrical boundary condition should favor the formation inside Ω of the positively magnetized phase; therefore, it will be natural to consider, in the canonical distribution, this boundary condition only when the total magnetization is fixed to be the spontaneous magnetization $m^*(\beta)$.

On the other hand, the $\pm$-boundary condition favors the separation of phases (positively magnetized phase near the top of Ω and negatively magnetized phase near the bottom). Therefore, it will be natural to consider the latter boundary condition in the case of a canonical distribution with magnetization $m = (1-2\alpha)m^*(\beta)$ with $0 < \alpha < 1$ ([51]). In the latter case, the positive phase can be expected to adhere to the top of Ω and to extend, in some sense to be discussed, up to a distance $O(L)$ from it; and then to change into the negatively magnetized pure phase.

To make the phenomenological description precise, consider the spin configurations $\boldsymbol{\sigma}$ through the associated sets of disjoint polygons (cf. the section "Symmetry-breaking phase transitions"). Fix the boundary conditions to be $++$ or $\pm$-cylindrical boundary conditions and note that polygons associated with a spin configuration $\boldsymbol{\sigma}$ are all closed and of two types: the ones of the first type, denoted $\gamma_1, \ldots, \gamma_n$, are polygons which do not encircle Ω; the second type of polygons, denoted by the symbols λ_α, are the ones which wind up, at least once, around Ω.

So, a spin configuration $\boldsymbol{\sigma}$ will be described by a set of polygons; the statistical weight of a configuration $\boldsymbol{\sigma} = (\gamma_1, \ldots, \gamma_n, \lambda_1, \ldots, \lambda_h)$ is (cf. [45]):

$$e^{-2\beta J\left(\sum_i |\gamma_i| + \sum_j |\lambda_j|\right)} \qquad [52]$$

The reason why the contours λ that go around the cylinder Ω are denoted by λ (rather than by γ) is that they "look like" open contours (see the section "Symmetry-breaking phase transitions") if one forgets that the opposite sides of Ω have to be identified. In the case of the $\pm$-boundary conditions then the number of polygons of λ-type must be odd (hence $\neq 0$), while for the $++$-boundary condition the number of λ-type polygons must be even (hence it could be 0).

For more details, the reader is referred to Sinai (1991) and Gallavotti (1999).

Separation and Coexistence of Phases

In the context of the geometric description of the spin configuration in the last section, consider the canonical distributions with $++$-cylindrical or the $\pm$-cylindrical boundary conditions and zero field: they will be denoted briefly as $\mu_{\beta,++}$, $\mu_{\beta,\pm}$, respectively. The following theorem (*Minlos–Sinai's theorem*) provided the foundations of the microscopic theory of coexistence: it is formulated in dimension $d=2$ but, modulo obvious changes, it holds for $d \geq 2$.

Theorem *For* $0 < \alpha < 1$ *fixed, let* $m = (1-2\alpha)\, m^*(\beta)$; *then for* β *large enough a spin configuration* $\boldsymbol{\sigma} = (\gamma_1, \ldots, \gamma_n, \lambda_1, \ldots, \lambda_{2h+1})$ *randomly chosen with the distribution* $\mu_{\beta,\pm}$ *enjoys the properties (i)–(iv) below with a* $\mu_{\beta,\pm}$*-probability approaching* 1 *as* $\Omega \to \infty$:

(i) $\boldsymbol{\sigma}$ *contains only one contour of* λ*-type and*

$$||\lambda| - (1+\varepsilon(\beta))L| < o(L) \qquad [53]$$

where $\varepsilon(\beta) > 0$ *is a suitable* (α*-independent*) *function of* β *tending to zero exponentially fast as* $\beta \to \infty$.

(ii) *If* $\Omega_\lambda^+, \Omega_\lambda^-$ *denote respectively, the regions above and below* λ, *and* $|\Omega| \equiv V, |\Omega^+|, |\Omega^-|$ *are, respectively, the volumes of* Ω, Ω^+, Ω^- *then*

$$\begin{aligned} &||\Omega_\lambda^+| - \alpha V| < \kappa(\beta)\, V^{3/4} \\ &|\Omega_\lambda^-| - (1-\alpha)V| < \kappa(\beta)\, V^{3/4} \end{aligned} \qquad [54]$$

where $\kappa(\beta) \xrightarrow[\beta\to\infty]{}$ *exponentially fast; the exponent* 3/4, *here and below, is not optimal.*

(iii) *If* $M_\lambda^+ = \sum_{x\in\Omega_\lambda^+} \sigma_x$ and $M_\lambda^- = \sum_{x\in\Omega_\lambda^-} \sigma_x$, *then*

$$\begin{aligned} &|M_\lambda^+ - \alpha m^*(\beta)\, V| < \kappa(\beta)\, V^{3/4} \\ &M_\lambda^- - (1-\alpha)\, m^*(\beta)\, V| < \kappa(\beta) V^{3/4} \end{aligned} \qquad [55]$$

(iv) *If* $K_\gamma^\lambda(\boldsymbol{\sigma})$ *denotes the number of contours congruent to a given* γ *and lying in* Ω_λ^+ *then, simultaneously for all the shapes of* γ:

$$|K_\gamma^\lambda(\boldsymbol{\sigma}) - \rho(\gamma)\alpha V| \leq Ce^{-\beta J|\gamma|} V^{1/2}, \quad C>0 \qquad [56]$$

where $\rho(\gamma) \leq e^{-2\beta J|\gamma|}$ *is the same quantity as already mentioned in the text of the theorem of "Finite-volume effects". A similar result holds for the contours below* λ (cf. *the comments on* [47]).

The above theorem not only provides a detailed and rather satisfactory description of the phase separation phenomenon, but it also furnishes a precise microscopic definition of the line of separation between the two phases, which should be naturally identified with the (random) line λ.

A similar result holds in the canonical distribution $\mu_{\beta,++,m^*(\beta)}$ where (i) is replaced by: no λ-type polygon is present, while (ii), (iii) become superfluous, and (iv) is modified in the obvious way. In other words, a typical configuration for the distribution the $\mu_{\beta,++,m^*(\beta)}$ has the same appearance as a typical configuration of the corresponding grand canonical ensemble with $(+)$-boundary condition (whose properties are described by the theorem given in the section "Beyond low temperatures (ferromagnetic Ising model").

For more details, see Sinai (1991) and Gallavotti (1999).

Phase Separation Line and Surface Tension

Continuing to refer to the nearest-neighbor Ising ferromagnet, the theorem of the last section means that, if β is large enough, then the microscopic line λ, separating the two phases, is almost straight (since $\varepsilon(\beta)$ is small). The deviations of λ from a straight line are more conveniently studied in the grand canonical distributions $\mu_\pm^0$ with boundary condition set to $+1$ in the upper half of $\partial\Omega$, vertical sites included, and to -1 in the lower half: this is illustrated in **Figure 2** (see the section "Symmetry-breaking phase transitions"). The results can be converted into very similar results for grand canonical distributions with $\pm$-cylindrical boundary conditions of the last section.

Define λ to be *rigid* if the probability that λ passes through the center of the box Ω (i.e., 0) does not tend to 0 as $\Omega \to \infty$; otherwise, it is *not rigid*.

The notion of rigidity distinguishes between the possibilities for the line λ to be "straight." The "excess" length $\varepsilon(\beta)L$ (see [53]) can be obtained in two ways: either the line λ is essentially straight (in the geometric sense) with a few "bumps" distributed with a density of order $\varepsilon(\beta)$ or, otherwise, it is only locally straight and with an important part of the excess length being gained through a small bending on a large length scale. In three dimensions a similar phenomenon is possible. Rigidity of λ, or its failure, can in principle be investigated by optical means;

there can be interference of coherent light scattered by macroscopically separated surface elements of λ only if λ is rigid in the above sense.

It has been rigorously proved that, the line λ is *not rigid* in dimension 2. And, at least at low temperature, the fluctuation of the middle point is of the order $O(\sqrt{L})$. In dimension 3 however, it has been shown that the surface λ is *rigid* at low enough temperature.

A deeper analysis is needed to study the shape of the separation surface under other conditions, for example, with + boundary conditions in a canonical distribution with magnetization intermediate between $\pm m^*(\beta)$. It involves, as a prerequisite, the definition and many properties of the surface tension between the two phases. Here only the definition of surface tension in the case of $\pm$-boundary conditions in the two-dimensional case will be mentioned. If $Z^{++}(\Omega, m^*(\beta))$ and $Z^{+-}(\Omega, m)$ are, respectively, the canonical partition functions for the $++$- and $\pm$-cylindrical boundary conditions the tension $\tau(\beta)$ is defined as

$$\beta\tau(\beta) = -\lim_{\Omega\to\infty} \frac{1}{L} \log \frac{Z^{+-}(\Omega, m)}{Z^{++}(\Omega, m^*(\beta))}$$

The limit can be shown to be α-independent for β large enough: the definition and its justification is based on the microscopic geometric description in the section "Geometry of phase co-existence." The definition can be naturally extended to higher dimension (and to more general non-nearest-neighbor models). If $d=2$, the tension τ can be exactly computed at all temperatures below criticality and is $\beta\tau(\beta) = 2\beta J + \log\tanh\beta J$.

More remarkably, the definition can be extended to define the surface tension $\tau(\beta, \boldsymbol{n})$ in the "direction $\boldsymbol{n}$," that is, when the boundary conditions are such that the line of separation is in the average orthogonal to the unit vector $\boldsymbol{n}$. In this way, if $d=2$ and $\alpha \in (0,1)$ is fixed, it can be proved that at low enough temperature the canonical distribution with + boundary conditions and intermediate magnetization $m = (1-2\alpha)m^*(\beta)$ has typical configurations containing a spin $-$ region of area $\sim\alpha V$; furthermore, if the container is rescaled to size $L=1$, the region will have a limiting shape filling an area α bounded by a smooth curve whose form is determined by the classical macroscopic *Wulff's theory* of the shape of crystals in terms of the surface tension $\tau(\boldsymbol{n})$.

An interesting question remains open in the three-dimensional case: it is conceivable that the surface, although rigid at low temperature, might become "loose" at a temperature $\tilde{T}_c$ smaller than the critical temperature T_c (the latter being defined as the highest temperature below which there are at least two pure phases). The temperature $\tilde{T}_c$, whose existence is rather well established in numerical experiments, would be called the "roughening transition" temperature. The rigidity of λ is connected with the existence of translationally non-invariant equilibrium states. The latter exist in dimension $d=3$, but not in dimension $d=2$, where the discussed nonrigidity of λ, established all the way to T_c, provides the intuitive reason for the absence of non-translation-invariant states. It has been shown that in $d=3$ the roughening temperature $\tilde{T}_c(\beta)$ necessarily cannot be smaller than the critical temperature of the two-dimensional Ising model with the same coupling.

Note that existence of translationally noninvariant equilibrium states is not necessary for the description of coexistence phenomena. The theory of the nearest-neighbor two-dimensional Ising model is a clear proof of this statement.

The reader is referred to Onsager (1944), van Beyeren (1975), Sinai (1991), Miracle-Solé (1995), Pfister and Velenik (1999), and Gallavotti (1999) for more details.

Critical Points

Correlation functions for a system with short-range interactions and in an equilibrium state (which is a pure phase) have cluster properties (see [22]): their physical meaning is that in a pure phase there is independence between fluctuations occurring in widely separated regions. The simplest cluster property concerns the "pair correlation function," that is, the probability density $\rho(\boldsymbol{q}_1, \boldsymbol{q}_2)$ of finding particles at points $\boldsymbol{q}_1, \boldsymbol{q}_2$ independently of where the other particles may happen to be (see [23]). In the case of spin systems, the pair correlation $\rho(\boldsymbol{q}_1, \boldsymbol{q}_2) = \langle \sigma_{q_1} \sigma_{q_2} \rangle$ will be considered. The pair correlation of a translation-invariant equilibrium state has a cluster property ([22], [42]), if

$$|\rho(\boldsymbol{q}_1, \boldsymbol{q}_2) - \rho^2| \xrightarrow[|q_1 - q_2|\to\infty]{} 0 \qquad [57]$$

where ρ is the probability density for finding a particle at $\boldsymbol{q}$ (i.e., the physical density of the state) or $\rho = \langle \sigma_q \rangle$ is the average of the value of the spin at $\boldsymbol{q}$ (i.e., the magnetization of the state).

A general definition of critical point is a point c in the space of the parameters characterizing equilibrium states, for example, β, λ in grand canonical distributions, β, v in canonical distributions, or β, h in the case of lattice spin systems in a grand canonical

distribution. In systems with short-range interaction (i.e., with $\varphi(r)$ vanishing for $|r|$ large enough) the point c is a critical point if the pair correlation tends to 0 (see [57]), slower than exponential (e.g., as a power of the distance $|r| = |q_1 - q_2|$).

A typical example is the two-dimensional Ising model on a square lattice and with nearest-neighbor ferromagnetic interaction of size J. It has a single critical point at $\beta = \beta_c$, $h = 0$ with $\sinh 2\beta_c J = 1$. The cluster property is that $\langle \sigma_x \sigma_y \rangle - \langle \sigma_x \rangle \langle \sigma_y \rangle \xrightarrow[|x-y| \to \infty]{} 0$ as

$$A_+(\beta) \frac{e^{-\kappa(\beta)|x-y|}}{\sqrt{|x-y|}}, \qquad A_-(\beta) \frac{e^{-\kappa(\beta)|x-y|}}{|x-y|^2}$$
$$A_c \frac{1}{|x-y|^{1/4}}, \qquad [58]$$

for $\beta < \beta_c$, $\beta > \beta_c$, or $\beta = \beta_c$, respectively, where $A_\pm(\beta)$, A_c, $\kappa(\beta) > 0$. The properties [58] stem from the exact solution of the model.

At the critical point, several interesting phenomena occur: the lack of exponential decay indicates lack of a length scale over which really distinct phenomena can take place, and properties of the system observed at different length scales are likely to be simply related by suitable scaling transformations. Many efforts have been dedicated at finding ways of understanding quantitatively the scaling properties pertaining to different observables. The result has been the development of the *renormalization group* approach to critical phenomena (cf. the section "Renormalization group"). The picture that emerges is that the closer the critical point is the larger becomes the maximal scale of length below which scaling properties are observed. For instance, in a lattice spin system in zero field the magnetization $M|\Lambda|^{-a}$ in a box $\Lambda \subset \Omega$ should have essentially the same distribution for all Λ's with side $< l_0(\beta)$ and $l_0(\beta) \to \infty$ as $\beta \to \beta_c$, provided a is suitably chosen. The number a is called a *critical exponent*.

There are several other "critical exponents" that can be defined near a critical point. They can be associated with singularities of the thermodynamic function or with the behavior of the correlation functions involving joint densities at two or more than two points. As an example, consider a lattice spin system: then the "$2n$–spins correlation" $\langle \sigma_0 \sigma_{\xi_1} \dots \sigma_{\xi_{2n-1}} \rangle_c$ could behave proportionally to $\chi_{2n}(0, \xi_1, \dots, \xi_{2n-1})$, $n = 1, 2, 3, \dots$, for a suitable family of homogeneous functions χ_n, of some degree ω_{2n}, of the coordinates $(\xi_1, \dots, \xi_{2n-1})$ at east when the reciprocal distances are large but $< l_0(\beta)$ and

$$l_0(\beta) = \text{const.}(\beta - \beta_c)^{-\nu} \underset{\beta \to \beta_0}{\longrightarrow} \infty$$

This means that if ξ_i are regarded as points in $\mathbb{R}^d$ there are functions χ_{2n} such that

$$\chi_{2n}\left(0, \frac{\xi_1}{\lambda}, \dots, \frac{\xi_{2n-1}}{\lambda}\right) = \lambda^{\omega_{2n}} \chi_{2n}(0, \xi_1, \dots, \xi_{2n-1})$$
$$0 < \lambda \in \mathbb{R} \qquad [59]$$

and $\langle \sigma_0 \sigma_{\xi_1} \dots \sigma_{\xi_{2n-1}} \rangle \propto \chi_{2n}(0, \xi_1, \dots, \xi_{2n-1})$ if $1 \ll |x_i - x_j| \ll l_0(\beta)$. The numbers ω_{2n} define a sequence of critical exponents.

Other critical exponents can be associated with approaching the critical point along other directions (e.g., along $h \to 0$ at $\beta = \beta_c$). In this case, the length up to which there are scaling phenomena is $l_0(h) = \ell_o h^{-\bar{\nu}}$. Further, the magnetization $m(h)$ tends to 0 as $h \to 0$ at fixed $\beta = \beta_c$ as $m(h) = m_0 h^{1/\delta}$ for $\delta > 0$.

None of the feautres of critical exponents is known rigorously, including their existence. An exception is the case of the two–dimensional nearest-neighbor Ising ferromagnet where some exponents are known exactly (e.g., $\omega_2 = 1/4$, $\omega_{2n} = n\omega_2$, or $\nu = 1$, while δ, $\bar{\nu}$ are not rigorously known). Nevertheless, for Ising ferromagnets (not even nearest-neighbor but, as always here, finite-range) in all dimensions, all of the exponents mentioned are conjectured to be the same as those of the nearest-neighbor Ising ferromagnet. A further exception is the derivation of rigorous relations between critical exponents and, in some cases, even their values under the assumption that they exist.

Remark Naively it could be expected that in a pure state in zero field with $\langle \sigma_x \rangle = 0$ the quantity $s = |\Lambda|^{-1/2} \sum_{x \in \Lambda} \sigma_x$, if Λ is a cubic box of side ℓ, should have a probability distribution which is Gaussian, with dispersion $\lim_{\Lambda \to \infty} \langle s^2 \rangle$. This is "usually true," but not always. Properties [58] show that in the $d = 2$ ferromagnetic nearest-neighbor Ising model, $\langle s^2 \rangle$ diverges proportionally to $\ell^{2-\frac{1}{4}}$ so that the variable s cannot have the above Gaussian distribution. The variable $S = |\Lambda|^{-7/8} \sum_{x \in \Lambda} \sigma_x$ will have a finite dispersion: however, there is no reason that it should be Gaussian. This makes clear the great interest of a fluctuation theory and its relevance for the critical point studies (see the next two sections).

For more details, the reader is referred to Onsager (1944), Domb and Green (1972), McCoy and Wu (1973), and Aizenman (1982).

Fluctuations

As it appears from the discussion in the last section, fluctuations of observables around their averages have interesting properties particularly at critical points. Of particular interest are observables that

are averages, over large volumes Λ, of local functions $F(x)$ on phase space: this is so because macroscopic observables often have this form. For instance, given a region Λ inside the system container Ω, $\Lambda \subset \Omega$, consider a configuration $x = (P, Q)$ and the number of particles $N_\Lambda = \sum_{q \in \Lambda} 1$ in Λ, or the potential energy $\Phi_\Lambda = \sum_{(q,q') \in \Lambda} \varphi(q - q')$ or the kinetic energy $K_\Lambda = \sum_{q \in \Lambda} (1/2m)p^2$. In the case of lattice spin systems, consider a configuration σ and, for instance, the magnetization $M_\Lambda = \sum_{i \in \Lambda} \sigma_i$ in Λ. Label the above four examples by $\alpha = 1, \ldots, 4$.

Let μ_α be the probability distribution describing the equilibrium state in which the quantities X_Λ are considered; let $x_\Lambda = \langle X_\Lambda/|\Lambda| \rangle_{\mu_\alpha}$ and $p \stackrel{\text{def}}{=} (X_\Lambda - x_\Lambda)/|\Lambda|$. Then typical properties of fluctuations that should be investigated are ($\alpha = 1, \ldots, 4$):

1. for all $\delta > 0$ it is $\lim_{\Lambda \to \infty} \mu_\alpha(|p| > \delta) = 0$ (*law of large numbers*);
2. there is $D_\alpha > 0$ such that

$$\mu(p\sqrt{|\Lambda|} \in [a, b]) \underset{\Lambda \to \infty}{\longrightarrow} \int_a^b \frac{dz}{\sqrt{2\pi D_\alpha}} e^{-z^2/2D_\alpha}$$

(*central limit law*); and

3. there is an interval $I_\alpha = (p^*_{\alpha,-}, p^*_{\alpha,+})$ and a concave function $F_\alpha(p)$, $p \in I$, such that if $[a, b] \subset I$ then

$$\frac{1}{|\Lambda|} \log \mu(p \in [a, b]) \underset{\Lambda \to \infty}{\longrightarrow} \max_{p \in [a,b]} F_\alpha(p)$$

(*large deviations law*).

The law of large numbers provides the certainty of the macroscopic values; the central limit law controls the small fluctuations (of order $\sqrt{|\Lambda|}$) of X_Λ around its average; and the large deviations law concerns the fluctuations of order $|\Lambda|$.

The relations (1)–(3) above are not always true: they can be proved under further general assumptions if the potential φ satisfies [14] in the case of particle systems or if $\sum_q |\varphi(q)| < \infty$ in the case of lattice spin systems. The function $F_\alpha(p)$ is defined in terms of the thermodynamic limits of suitable thermodynamic functions associated with the equilibrium state μ_α. The further assumption is, essentially in all cases, that a suitable thermodynamic function in terms of which $F_\alpha(p)$ will be expressed is smooth and has a nonvanishing second derivative.

For the purpose of a simple concrete example, consider a lattice spin system of Ising type with energy $-\sum_{x,y \in \Omega} \varphi(x - y)\sigma_x\sigma_y - \sum_x h\sigma_x$ and the fluctuations of the magnetization $M_\Lambda = \sum_{x \in \Lambda} \sigma_x$, $\Lambda \subset \Omega$, in the grand canonical equilibrium states $\mu_{h,\beta}$.

Let the free energy be $\beta f(\beta, h)$ (see [41]), let $m = m(h) \stackrel{\text{def}}{=} \langle M_\Lambda/|\Lambda| \rangle$ and let $h(m)$ be the inverse function of $m(h)$. If $p = M_\Lambda/|\Lambda|$ the function $F(p)$ is given by

$$F(p) = \beta(f(\beta, h(p)) - f(\beta, h) - \partial_h f(\beta, h)(h(p) - h)) \quad [60]$$

then a quite general result is:

Theorem *The relations* (1)–(3) *hold if the potential satisfies* $\sum_x |\varphi(x)| < \infty$ *and if* $F(p)$ [60] *is smooth and* $F''(p) \neq 0$ *in open intervals around those in which* p *is considered, that is, around* $p = 0$ *for the law of large numbers and for the central limit law or in an open interval containing* a, b *for the case of the large deviations law.*

In the cases envisaged, the theory of equivalence of ensembles implies that the function F can also be computed via thermodynamic functions naturally associated with other equilibrium ensembles. For instance, instead of the grand canonical $f(\beta, h)$, one could consider the canonical $\beta g(\beta, m)$ (see [41]), then

$$F(p) = -\beta(g(\beta, p) - g(\beta, m) - \partial_m g(\beta, m)(p - m)) \quad [61]$$

It has to be remarked that there should be a strong relation between the central limit law and the law of large deviations. Setting aside stating the conditions for a precise mathematical theorem, the statement can be efficiently illustrated in the case of a ferromagnetic lattice spin system and with $\Lambda \equiv \Omega$, by showing that the law of large deviations in small intervals, around the average $m(h_0)$, at a value h_0 of the external field, is implied by the validity of the central limit law for all values of h near h_0 and vice versa (here β is fixed). Taking $h_0 = 0$ (for simplicity), the heuristic reasons are the following. Let $\mu_{h,\Omega}$ be the grand canonical distribution in external field h. Then:

1. The probability $\mu_{h,\Omega}(p \in dp)$ is proportional, by definition, to $\mu_{0,\Omega}(p \in dp)e^{-\beta hp|\Omega|}$. Hence, if the central limit law holds for all h near $h_0 = 0$, there will exist two functions $m(h)$ and $D(h) > 0$, defined for h near $h_0 = 0$, with $m(0) = 0$ and

$$\mu_0(p \in dp)e^{-\beta hp|\Omega|} = \text{const.} \exp\left(-|\Omega| \frac{(p - m(h))^2}{2D(h)} + o(\Omega)\right) dp \quad [62]$$

2. There is a function $\zeta(m)$ such that $\partial_m \zeta(m(h)) = \beta h$ and $\partial_m^2 \zeta(m(h)) = D(h)^{-1}$. (This is obtained by noting that, given $D(h)$, the differential equation $\partial_m \beta h = D(h)^{-1}$ with the initial value $h(0) = 0$ determines the function $h(m)$; therefore, $\zeta(m)$ is determined by a second integration, from $\partial_m \zeta(m) = \beta h(m)$.

It then follows, heuristically, that the probability of p in zero field has the form const. $e^{\zeta(p)|\Omega|}\,dp$ so that the probability that $p \in [a,b]$ will be const $\exp(|\Omega| \max_{p\in[a,b]} \zeta(p))$.

Conversely, the large deviations law for p at $h=0$ implies the validity of the central limit law for the fluctuations of p in all small enough fields h: this simply arises from the function $F(p)$ having a negative second derivative.

This means that there is a "duality" between central limit law and large deviation law or that the law of large deviations is a "global version" of the central limit law, in the sense that:

1. if the central limit law holds for h in an interval around h_0 then the fluctuations of the magnetization at field h_0 satisfy a large deviation law in a small enough interval J around $m(h_0)$; and
2. if a large deviation law is satisfied in an interval around h_0 then the central limit law holds for the fluctuations of magnetization around its average in all fields h with $h - h_0$ small enough.

Going beyond the heuristic level in establishing the duality amounts to giving a precise meaning to "small enough" and to discuss which properties of $m(h)$ and $D(h)$, or $F(p)$ are needed to derive properties (1), (2).

For purposes of illustration consider the Ising model with ferromagnetic short range interaction φ: then the central limit law holds for all h if β is small enough and, under the same condition on β, the large deviations law holds for all h and all intervals $[a,b] \subset (-1,1)$. If β is not small then the condition $h \neq 0$ has to be added. Hence, the conditions are fairly weak and the apparent exceptions concern the value $h=0$ and β not small where the statements may become invalid because of possible phase transitions.

In presence of phase transitions, the law of large numbers, the central limit law, and law of large deviations should be reformulated. Basically, one has to add the requirement that fluctuations are considered in pure phases and change, in a natural way, the formulation of the laws. For instance, the large fluctuations of magnetization in a pure phase of the Ising model in zero field and large β (i.e., in a state obtained as limit of finite-volume states with + or − boundary conditions) in intervals $[a,b]$ which do not contain the average magnetization m^* are not necessarily exponentially small with the size of $|\Lambda|$: if $[a,b] \subset [-m^*, m^*]$ they are exponentially small but only with the size of the surface of Λ (i.e., with $|\Lambda|^{(d-1)/d}$) while they are exponentially small with the volume if $[a,b] \cap [-m^*, m^*] = \emptyset$.

The discussion of the last section shows that at the critical point the nature of the large fluctuations is also expected to change: no central limit law is expected to hold in general because of the example of [58] with the divergence of the average of the normal second moment of the magnetization in a box as the side tends to ∞.

For more details the reader is referred to Olla (1987).

Renormalization Group

The theory of fluctuations just discussed concerns only fluctuations of a single quantity. The problem of joint fluctuations of several quantities is also interesting and in fact led to really new developments in the 1970s. It is necessary to restrict attention to rather special cases in order to illustrate some ideas and the philosophy behind the approach. Consider, therefore, the equilibrium distribution μ_0 associated with one of the classical equilibrium ensembles. To fix the ideas we consider the equilibrium distribution of an Ising energy function βH_0, having included the temperature factor in the energy: the inclusion is done because the discussion will deal with the properties of μ_0 as a function of β. It will also be assumed that the average of each spin is zero ("no magnetic field," see [39] with $h=0$). Keeping in mind a concrete case, imagine that βH_0 is the energy function of the nearest-neighbor Ising ferromagnet in zero field.

Imagine that the volume Ω of the container has periodic boundary conditions and is very large, ideally infinite. Define the family of blocks $k\boldsymbol{\xi}$, parametrized by $\boldsymbol{\xi} \in \mathbb{Z}^d$ and with k an integer, consisting of the lattice sites $\boldsymbol{x} = \{k\xi_i \leq x_i < (k+1)\xi_i\}$. This is a lattice of cubic blocks with side size k that will be called the "k-rescaled lattice."

Given α, the quantities $m_{\boldsymbol{\xi}} = k^{-\alpha d} \sum_{x \in k\boldsymbol{\xi}} \sigma_x$ are called the block spins and define the map $R^*_{\alpha,k}\mu_0 = \mu_k$ transforming the initial distribution on the original spins into the distribution of the block spins. Note that if the initial spins have only two values $\sigma_x = \pm 1$, the block spins take values between $-k^d/k^{\alpha d}$ and $k^d/k^{\alpha d}$ at steps of size $2/k^{\alpha d}$. Furthermore, the map $R^*_{\alpha,k}$ makes sense independently of how many values the initial spins can assume, and even if they assume a continuum of values $S_x \in \mathbb{R}$.

Taking $\alpha = 1$ means, for k large, looking at the probability distribution of the joint large fluctuations in the blocks $k\boldsymbol{\xi}$. Taking $\alpha = 1/2$ corresponds to studying a joint central limit property for the block variables.

Considering a one-parameter family of initial distributions μ_0 parametrized by a parameter β

(that will be identified with the inverse temperature), typically there will be a unique value $\alpha(\beta)$ of α such that the joint fluctuations of the block variables admit a limiting distribution,

$$\text{prob}_k(m_\xi \in [a_\xi, b_\xi], \sigma \in \Lambda) \underset{k\to\infty}{\longrightarrow} \int_{\{a_\xi\}}^{\{b_\xi\}} g_\Lambda((S_\xi)_{\xi\in\Lambda}) \prod_{\xi\in\Lambda} dS_\xi \qquad [63]$$

for some distribution $g_\Lambda(z)$ on $\mathbb{R}^\Lambda$.

If $\alpha > \alpha(\beta)$, the limit will then be $\prod_{\xi\in\Lambda} \delta(S_\xi)\, dS_\xi$, or if $\alpha < \alpha(\beta)$ the limit will not exist (because the block variables will be too large, with a dispersion diverging as $k \to \infty$).

It is convenient to choose as sequence of $k \to \infty$ the sequence $k = 2^n$ with $n = 0, 1, \ldots$ because in this way it is $R^*_{\alpha,k} \equiv R^{*n}_{\alpha,1}$ and the limits $k \to \infty$ along the sequence $k = 2^n$ can be regarded as limits on a sequence of iterations of a map $R^*_{\alpha,1}$ acting on the probability distributions of generic spins S_x on the lattice $\mathbb{Z}^d$ (the sequence 3^n would be equally suited).

It is even more convenient to consider probability distributions that are expressed in terms of energy functions H which generate, in the thermodynamic limit, a distribution μ: then $R^*_{\alpha,1}$ defines an action R_α on the energy functions so that $R_\alpha H = H'$ if H generates μ, H' generates μ' and $R^*_{\alpha,1}\mu = \mu'$. Of course, the energy function will be more general than [39] and at least a form like δU in [49] has to be admitted.

In other words, R_α gives the result of the action of $R^*_{\alpha,1}$ expressed as a map acting on the energy functions. Its iterates also define a semigroup which is called the block spin renormalization group.

While the map $R^*_{\alpha,1}$ is certainly well defined as a map of probability distributions into probability distributions, it is by no means clear that R_α is well defined as a map on the energy functions. Because, if μ is given by an energy function, it is not clear that $R^*_{\alpha,1}\mu$ is such.

A remarkable theorem can be (easily) proved when $R^*_{\alpha,1}$ and its iterates act on initial μ_0's which are equilibrium states of a spin system with short-range interactions and at high temperature (β small). In this case, if $\alpha = 1/2$, the sequence of distributions $R^{*n}_{1/2,1}\mu_0(\beta)$ admits a limit which is given by a product of independent Gaussians:

$$\text{prob}_k(m_\xi \in [a_\xi, b_\xi], \sigma \in \Lambda) \underset{k\to\infty}{\longrightarrow} \int_{\{a_\xi\}}^{\{b_\xi\}} \prod_{\xi\in\Lambda} \exp\left(-\frac{1}{2D(\beta)} S_\xi^2\right) \prod_{\xi\in\Lambda} \frac{dS_\xi}{\sqrt{2\pi D(\beta)}} \qquad [64]$$

Note that this theorem is stated without even mentioning the renormalization maps $R^n_{1/2}$: it can nevertheless be interpreted as stating that

$$R^n_{1/2}\beta H_0 \underset{n\to\infty}{\longrightarrow} \sum_{\xi\in\mathbb{Z}^d} \frac{1}{2D(\beta)} S_\xi^2 \qquad [65]$$

but the interpretation is not rigorous because [64] does not state require that $R^n_{1/2}H_0(\beta)$ makes sense for $n \geq 1$. It states that at high temperature block spins have normal independent fluctuations: it is therefore an extension of the central limit law.

There are a few cases in which the map R_α can be rigorously shown to be well defined at least when acting on special equilibrium states like the high-temperature lattice spin systems: but these are exceptional cases of relatively little interest.

Nevertheless, there is a vast literature dealing with approximate representations of the map R_α. The reason is that, assuming not only its existence but also that it has the properties that one would normally expect to hold for a map acting on a finite dimensional space, it follows that a number of consequences can be drawn; quite nontrivial ones as they led to the first theory of the critical point that goes beyond the van der Waals theory discribed in the section "van der Waals theory."

The argument proceeds essentially as follows. At the critical point, the fluctuations are expected to be anomalous (cf. the last remark in the section "Critical points") in the sense that $\langle (\sum_{x\in\Lambda} \sigma_\xi / \sqrt{|\Lambda|})^2 \rangle$ will tend to ∞, because $\alpha = 1/2$ does not correspond to the right fluctuation scale of $\sum_{\xi\in\Lambda} \sigma_\xi$, signaling that $R^{*n}_{1/2,1}\mu_0(\beta_c)$ will not have a limit but, possibly, there is $\alpha_c > 1/2$ such that $R^{*n}_{\alpha_c,1}\mu_0(\beta_c)$ converges to a limit in the sense of [63]. In the case of the critical nearest-neighbor Ising ferromagnetic $\alpha_c = 7/8$ (see ending remark in the section "Critical points"). Therefore, if the map $R^*_{\alpha_c,1}$ is considered as acting on $\mu_0(\beta)$, it will happen that for all $\beta < \beta_c$, $R^{*n}_{\alpha_c,1}\mu_0(\beta_c)$ will converge to a trivial limit $\prod_{\xi\in\Lambda} \delta(S_\xi)\, dS_\xi$ because the value α_c is greater than 1/2 while normal fluctuations are expected.

If the map R_{α_c} can be considered as a map on the energy functions, this says that $\prod_{\xi\in\Lambda} \delta(S_\xi)\, dS_\xi$ is a "(trivial) fixed point of the renormalization group" which "attracts" the energy functions βH_0 corresponding to the high-temperature phases.

The existence of the critical β_c can be associated with the existence of a *nontrivial fixed point* H^* for R_{α_c} which is hyperbolic with just one Lyapunov exponent $\lambda > 1$; hence, it has a stable manifold of codimension 1. Call μ^* the probability distribution corresponding to H^*.

The migration towards the trivial fixed point for $\beta < \beta_c$ can be explained simply by the fact that for

such values of β the initial energy function βH_0 is outside the stable manifold of the nontrivial fixed point and under application of the renormalization transformation $R^n_{\alpha_c}$, βH_0 migrates toward the trivial fixed point, which is attractive in all directions.

By increasing β, it may happen that, for $\beta = \beta_c$, βH_0 crosses the stable manifold of the nontrivial fixed point H^* for R_{α_c}. Then $R^n_{\alpha_c}\beta_c H_0$ will no longer tend to the trivial fixed point but it will tend to H^*: this means that the block spin variables will exhibit a completely different fluctuation behavior. If β is close to β_c, the iterations of R_{α_c} will bring $R^n_{\alpha_c}\beta H_0$ close to H^*, only to be eventually repelled along the unstable direction reaching a distance from it increasing as $\lambda^n|\beta - \beta_c|$.

This means that up to a scale length $O(2^{n(\beta)})$ lattice units with $\lambda^{n(\beta)}|\beta - \beta_c| = 1$ (i.e., up to a scale $O(|\beta - \beta_c|^{-\log_2 \lambda})$), the fluctuations will be close to those of the fixed point distribution μ^*, but beyond that scale they will come close to those of the trivial fixed point: to see them the block spins would have to be normalized with index $\alpha = 1/2$ and they would appear as uncorrelated Gaussian fluctuations (cf. [64], [65]).

The next question concerns finding the nontrivial fixed points, which means finding the energy functions H^* and the corresponding α_c which are fixed points of R_{α_c}. If the above picture is correct, the distributions μ^* corresponding to the H^* would describe the critical fluctuations and, if there was only one choice, or a limited number of choices, of α_c and H^* this would open the way to a universality theory of the critical point hinted already by the "primitive" results of van der Waals' theory.

The initial hope was, perhaps, that there would be a very small number of critical values α_c and H^* possible: but it rapidly faded away leaving, however, the possibility that the critical fluctuations could be classified into universality classes. Each class would contain many energy functions which, upon iterated actions of R_{α_c}, would evolve under the control of the trivial fixed point (always existing) for β small while, for $\beta = \beta_c$, they would be controlled, instead, by a nontrivial fixed point H^* for R_{α_c} with the same α_c and the same H^*. For $\beta < \beta_c$, a "resolution" of the approach to the trivial fixed point would be seen by considering the map $R_{1/2}$ rather than R_{α_c} whose iterates would, however, lead to a Gaussian distribution like [64] (and to a limit energy function like [65]).

The picture is highly hypothetical: but it is the first suggestion of a mechanism leading to critical points with the character of universality and with exponents different from those of the van der Waals theory or, for ferromagnets on a lattice, from those of its lattice version (the *Curie–Weiss theory*). Furthermore, accepting the approximations (e.g., the Wilson–Fisher ε-expansion) that allow one to pass from the well-defined $R^*_{\alpha,1}$ to the action of R_α on the energy functions, it is possible to obtain quite unambiguously values for α_c and expressions for H^* which are associated with the action of R_{α_c} on various classes of models.

For instance, it can lead to conclude that the critical behavior of all ferromagnetic finite-range lattice spin systems (with energy functions given by [39]) have critical points controlled by the same α_c and the same nontrivial fixed point: this property is far from being mathematically proved, but it is considered a major success of the theory. One has to compare it with van der Waals' critical point theory: *for the first time*, an approximation scheme has led, even though under approximations not fully controllable, to computable critical exponents which are not equal to those of the van der Waals theory.

The renormalization group approach to critical phenomena has many variants, depending on which kind of fluctuations are considered and on the models to which it is applied. In statistical mechanics, there are a few mathematically complete applications: certain results in higher dimensions, theory of dipole gas in $d = 2$, hierarchical models, some problems in condensed matter and in statistical mechanics of lattice spins, and a few others. Its main mathematical successes have occured in various related fields where not only the philosophy described above can be applied but it leads to renormalization transformations that can be defined precisely and studied in detail: for example, constructive field theory, KAM theory of quasiperiodic motions, and various problems in dynamical systems.

However, the applications always concern special cases and in each of them the general picture of the trivial–nontrivial fixed point dichotomy appears realized but without being accompanied, except in rare cases (like the hierarchical models or the universality theory of maps of the interval), by the full description of stable manifold, unstable direction, and action of the renormalization transformation on objects other than the one of immediate interest (a generality which looks often an intractable problem, but which also turns out not to be necessary).

In the renormalization group context, mathematical physics has played an important role also by providing clear evidence that universality classes could not be too few: this was shown by the numerous exact solutions after Onsager's solution of the nearest-neighbor Ising ferromagnet: there are in fact several lattice models in $d = 2$ that exhibit critical points with some critical exponents exactly computable and that depend continuously on the models parameters.

For more details, we refer the reader to McCoy and Wu (1973), Baxter (1982), Bleher and Sinai (1975), Wilson and Fisher (1972), Gawedzky and Kupiainen (1983, 1985), Benfatto and Gallavotti (1995), and Mastropietro (2004).

Quantum Statistics

Statistical mechanics is extended to assemblies of quantum particles rather straightforwardly. In the case of N identical particles, the observables are operators O on the Hilbert space

$$\mathcal{H}_N = L_2(\Omega)^N_\alpha \quad \text{or} \quad \mathcal{H}_N = (L_2(\Omega)\otimes \mathcal{C}^2)^N_\alpha$$

where $\alpha = +, -$, of the symmetric ($\alpha = +$, bosonic particles) or antisymmetric ($\alpha = -$, fermionic particles) functions $\psi(\boldsymbol{Q})$, $\boldsymbol{Q} = (\boldsymbol{q}_1, \ldots, \boldsymbol{q}_N)$, of the position coordinates of the particles or of the position and spin coordinates $\psi(\boldsymbol{Q}, \boldsymbol{\sigma})$, $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_N)$, normalized so that

$$\int |\psi(\boldsymbol{Q})|^2 \, \mathrm{d}\boldsymbol{Q} = 1 \quad \text{or} \quad \sum_{\boldsymbol{\sigma}} \int |\psi(\boldsymbol{Q}, \boldsymbol{\sigma})|^2 \, \mathrm{d}\boldsymbol{Q} = 1$$

here only $\sigma_j = \pm 1$ is considered. As in classical mechanics, a state is defined by the average values $\langle O \rangle$ that it attributes to the observables.

Microcanonical, canonical, and grand canonical ensembles can be defined quite easily. For instance, consider a system described by the Hamiltonian ($\hbar$ = Planck's constant)

$$H_N = -\frac{\hbar^2}{2m}\sum_{j=1}^{N} \Delta_{\boldsymbol{q}_j} + \sum_{j<j'} \varphi(\boldsymbol{q}_j - \boldsymbol{q}_{j'}) + \sum_j w(\boldsymbol{q}_j)$$

$$\stackrel{\text{def}}{=} K + \boldsymbol{\Phi} \qquad [66]$$

where periodic boundary conditions are imagined on Ω and $w(\boldsymbol{q})$ is periodic, smooth potential (the side of Ω is supposed to be a multiple of the periodic potential period if $w \neq 0$). Then a canonical equilibrium state with inverse temperature β and specific volume $v = V/N$ attributes to the observable O the average value

$$\langle O \rangle \stackrel{\text{def}}{=} \frac{\operatorname{tr} \mathrm{e}^{-\beta H_N} O}{\operatorname{tr} \mathrm{e}^{-\beta H_N}} \qquad [67]$$

Similar definitions can be given for the grand canonical equilibrium states.

Remarkably, the ensembles are orthodic and a "heat theorem" (see the section "Heat theorem and ergodic hypothesis") can be proved. However, "equipartition" does not hold: that is, $\langle K \rangle \neq (d/2)N\beta^{-1}$, although β^{-1} is still the integrating factor of $\mathrm{d}U + p\,\mathrm{d}V$ in the heat theorem; hence, β^{-1} continues to be proportional to temperature.

Lack of equipartition is important, as it solves paradoxes that arise in classical statistical mechanics applied to systems with infinitely many degrees of freedom, like crystals (modeled by lattices of coupled oscillators) or fields (e.g., the electromagnetic field important in the study of black body radiation). However, although this has been the first surprise of quantum statistics (and in fact responsible for the very discovery of quanta), it is by no means the last.

At low temperatures, new unexpected (i.e., with no analogs in classical statistical mechanics) phenomena occur: Bose–Einstein condensation (superfluidity), Fermi surface instability (superconductivity), and appearance of off-diagonal long-range order (ODLRO) will be selected to illustrate the deeply different kinds of problems of quantum statistical mechanics. Largely not yet understood, such phenomena pose very interesting problems not only from the physical point of view but also from the mathematical point of view and may pose challenges even at the level of a definition. However, it should be kept in mind that in the interesting cases (i.e., three-dimensional systems and even most two- and one-dimensional systems) there is no proof that the objects defined below really exist for the systems like [66] (see, however, the final comment for an important exception).

Bose–Einstein Condensation

In a canonical state with parameters β, v, a definition of the occurrence of Bose condensation is in terms of the eigenvalues $\nu_j(\Omega, N)$ of the kernel $\rho(\boldsymbol{q}, \boldsymbol{q}')$ on $L_2(\Omega)$, called the *one-particle reduced density matrix*, defined by

$$N\sum_{n=1}^{\infty} \frac{\mathrm{e}^{-\beta E_n(\Omega,N)}}{\operatorname{tr} \mathrm{e}^{-\beta H_N}} \int \bar{\psi}_n(\boldsymbol{q}, \boldsymbol{q}_1, \ldots, \boldsymbol{q}_{N-1}) \times \psi_n(\boldsymbol{q}', \boldsymbol{q}_1, \ldots, \boldsymbol{q}_{N-1}) \, \mathrm{d}\boldsymbol{q}_1 \ldots \mathrm{d}\boldsymbol{q}_{N-1} \qquad [68]$$

where $E_n(\Omega, N)$ are the eigenvalues of H_N and $\psi_n(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_N)$ are the corresponding eigenfunctions. If ν_j are ordered by increasing value, the state with parameters β, v is said to contain a *Bose–Einstein condensate* if $\nu_1(\Omega, N) \geq bN > 0$ for all large Ω at $v = V/N, \beta$ fixed. This receives the interpretation that there are more than bN particles with equal momentum. The free Bose gas exhibits a Bose condensation phenomenon at fixed density and small temperature.

Fermi Surface

The wave functions $\psi_n(\boldsymbol{q}_1, \sigma_1, \ldots, \boldsymbol{q}_N, \sigma_N) \equiv \psi_n(\boldsymbol{Q}, \boldsymbol{\sigma})$ are now antisymmetric in the permutations of the pairs $(\boldsymbol{q}_i, \sigma_i)$. Let $\psi(\boldsymbol{Q}, \boldsymbol{\sigma}; N, n)$ denote the nth

eigenfunction of the N-particle energy H_N in [66] with eigenvalue $E(N,n)$ (labeled by $n=0,1,\ldots$ and non-decreasingly ordered). Setting $\boldsymbol{Q}''=(\boldsymbol{q}_1'',\ldots,\boldsymbol{q}_{N-p}'')$, $\boldsymbol{\sigma}''=(\sigma_1'',\ldots,\sigma_{N-p}'')$, introduce the kernels $\rho_p^{H_N}(\boldsymbol{Q},\boldsymbol{\sigma};\boldsymbol{Q}',\boldsymbol{\sigma}')$ by

$$\rho_p(\boldsymbol{Q},\boldsymbol{\sigma};\boldsymbol{Q}',\boldsymbol{\sigma}') \stackrel{\text{def}}{=} p!\binom{N}{p}\int \sum_{\boldsymbol{\sigma}''} \mathrm{d}^{N-p}\boldsymbol{Q}'' \sum_{n=0}^{\infty} \frac{\mathrm{e}^{-\beta E(N,n)}}{\operatorname{tr}\mathrm{e}^{-\beta H_N}} \times \overline{\psi}(\boldsymbol{Q},\boldsymbol{\sigma};\boldsymbol{Q}'',\boldsymbol{\sigma}'';N,n)\psi(\boldsymbol{Q}',\boldsymbol{\sigma}';\boldsymbol{Q}'',\boldsymbol{\sigma}'';N,n) \quad [69]$$

which are called *p-particle reduced density matrices* (extending the corresponding one-particle reduced density matrix [68]). Denote $\rho(\boldsymbol{q}_1-\boldsymbol{q}_2)\stackrel{\text{def}}{=}\sum_\sigma \rho_1(\boldsymbol{q}_1,\sigma,\boldsymbol{q}_2,\sigma)$. It is also useful to consider spinless fermionic systems: the corresponding definitions are obtained simply by suppressing the spin labels and will not be repeated.

Let $r_1(\boldsymbol{k})$ be the Fourier transform of $\rho_1(\boldsymbol{q}-\boldsymbol{q}')$: the Fermi surface can be defined as the locus of the $\boldsymbol{k}$'s in the neighborhood of which $\partial_{\boldsymbol{k}} r_1(\boldsymbol{k})$ is unbounded as $\Omega\to\infty$, $\beta\to\infty$. The limit as $\beta\to\infty$ is important because the notion of a Fermi surface is, possibly, precise only at zero temperature, that is at $\beta=\infty$.

So far, existence of Fermi surface (i.e., the smoothness of $r_1(\boldsymbol{k})$ except on a smooth surface in $\boldsymbol{k}$-space) has been proved in free Fermi systems ($\varphi=0$) and

1. certain exactly soluble one-dimensional spinless systems and
2. in rather general one-dimensional spinless systems or systems with spin and repulsive pair interaction, possibly in an external periodic potential.

The spinning case in a periodic potential and dimension $d\geq 2$ is the most interesting case to study for its relevance in the theory of conduction in crystals. Essentially no mathematical results are available as the above-mentioned ones do not concern any case in dimension >1: this is a rather deceiving aspect of the theory and a challenge.

In dimension 2 or higher, for fermionic systems with Hamiltonian [66], not only there are no results available, even without spin, but it is not even clear that a Fermi surface can exist in presence of interesting interactions.

Cooper Pairs

The superconductivity theory has been phenomenologically related to the existence of Cooper pairs. Consider the Hamiltonian [66] and define (cf. [69])

$$\rho(\boldsymbol{x}-\boldsymbol{y},\sigma;\boldsymbol{x}'-\boldsymbol{y}',\sigma';\boldsymbol{x}-\boldsymbol{x}') \stackrel{\text{def}}{=} \rho_2(\boldsymbol{x},\sigma,\boldsymbol{y},-\sigma;\boldsymbol{x}',\sigma',\boldsymbol{y}',-\sigma')$$

The system is said to contain *Cooper pairs* with spins $\sigma,-\sigma$ ($\sigma=+$ or $\sigma=-$) if there exist functions $g^\alpha(\boldsymbol{q},\sigma)\neq 0$ with

$$\int \overline{g^\alpha}(\boldsymbol{q},\sigma)g^{\alpha'}(\boldsymbol{q},\sigma)\,\mathrm{d}\boldsymbol{q}=0 \quad \text{if } \alpha\neq\alpha'$$

such that

$$\lim_{V\to\infty}\rho(\boldsymbol{x}-\boldsymbol{y},\sigma,\boldsymbol{x}'-\boldsymbol{y}',\sigma',\boldsymbol{x}-\boldsymbol{x}') \xrightarrow[\boldsymbol{x}-\boldsymbol{x}'\to\infty]{} \sum_\alpha g^\alpha(\boldsymbol{x}-\boldsymbol{y},\sigma)\overline{g^\alpha}(\boldsymbol{x}'-\boldsymbol{y}',\sigma') \quad [70]$$

In this case, $g^\alpha(\boldsymbol{x}-\boldsymbol{y},\sigma)$ with largest L_2 norm can be called, after normalize, the wave function of the paired state of lowest energy: this is the analog of the plane wave for a free particle (and, like it, it is manifestly not normalizable, i.e., it is not square integrable as a function of $\boldsymbol{x},\boldsymbol{y}$). If the system contains Cooper pairs and the nonleading terms in the limit [70] vanish quickly enough the two-particle reduced density matrix [70] regarded as a kernel operator has an eigenvalue of order V as $V\to\infty$: that is, the state of lowest energy is "macroscopically occupied," quite like the free Bose condensation in the ground state.

Cooper pairs instability might destroy the Fermi surface in the sense that $r_1(\boldsymbol{k})$ becomes analytic in $\boldsymbol{k}$; but it is also possible that, even in the presence of them, there remains a surface which is the locus of the singularities of the function $r_1(\boldsymbol{k})$. In the first case, there should remain a trace of it as a very steep gradient of $r_1(\boldsymbol{k})$ of the order of an exponential in the inverse of the coupling strength; this is what happens in the *BCS model* for superconductivity. The model is, however, a mean-field model and this particular regularity aspect might be one of its peculiarities. In any event, a smooth singularity surface is very likely to exist for some interesting density matrix (e.g., in the BCS model with "gap parameter γ" the wave function

$$g(\boldsymbol{x}-\boldsymbol{y},\sigma)\equiv\frac{1}{(2\pi)^d}\int_{\varepsilon(\boldsymbol{k})>0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})}\frac{\gamma}{\sqrt{\varepsilon(\boldsymbol{k})^2+\gamma^2}}\mathrm{d}\boldsymbol{k}$$

of the lowest energy level of the Cooper pairs is singular on a surface coinciding with the Fermi surface of the free system).

ODLRO

Consider the k-fermion reduced density matrix $\rho_k(\boldsymbol{Q},\boldsymbol{\sigma};\boldsymbol{Q}',\boldsymbol{\sigma}')$ as kernel operators O_k on $L_2((\Omega\times\mathcal{C}^2)^k)_-$. Suppose k is even, then if O_k has a (generalized) eigenvalue of order $N^{k/2}$ as $N\to\infty, N/V=\rho$, the system is said to exhibit *off-diagonal long-range* order of order k. For k odd, ODLRO is defined to exist if O_k has an eigenvalue of order $N^{(k-1)/2}$ and $k\geq 3$ (if $k=1$ the largest eigenvalue of O_1 is necessarily ≤ 1).

For bosons, consider the reduced density matrix $\rho_k(Q;Q')$ regarding it as a kernel operator O_k on $L_2(\Omega)^k_+$ and define ODLRO of order k to be present if $O(k)$ has a (generalized) eigenvalue of order N^k as $N \to \infty, N/V = \rho$.

ODLRO can be regarded as a unification of the notions of Bose condensation and of the existence of Cooper pairs, because Bose condensation could be said to correspond to the kernel operator $\rho_1(q_1 - q_2)$ in [68] having a (generalized) eigenvalue of order N, and to be a case of ODLRO of order 1. If the state is pure in the sense that it has a cluster property (see the sections "Phase transitions and boundary conditions" and "Lattice models"), then the existence of ODLRO, Bose condensation, and Cooper pairs implies that the system shows a spontaneously broken symmetry: conservation of particle number and clustering imply that the off-diagonal elements of (all) reduced density matrices vanish at infinite separation in states obtained as limits of states with periodic boundary conditions and Hamiltonian [66], and this is incompatible with ODLRO.

The free Fermi gas has no ODLRO, the BCS model of superconductivity has Cooper pairs and ODLRO with $k=2$, but no Fermi surface in the above sense (possibly too strict). Fermionic systems cannot have ODLRO of order 1 (because the reduced density matrix of order 1 is bounded by 1).

The contribution of mathematical physics has been particularly effective in providing exactly soluble models: however, the soluble models deal with one-dimensional systems and it can be shown that in dimensions 1, 2 no ODLRO can take place. A major advance is the recent proof of ODLRO and Bose condensation in the case of a lattice version of [66] at a special density value (and $d \geq 3$).

In no case, for the Hamiltonian [66] with $\varphi \neq 0$, existence of Cooper pairs has been proved nor existence of a Fermi surface for $d > 1$. Nevertheless, both Bose condensation and Cooper pairs formation can be proved to occur rigorously in certain limiting situations. There are also a variety of phenomena (e.g., simple spectral properties of the Hamiltonians) which are believed to occur once some of the above-mentioned ones do occur and several of them can be proved to exist in concrete models.

If $d=1,2$, ODLRO can be proved to be impossible at $T>0$ through the use of Bogoliubov's inequality (used in the "no $d=2$ crystal theorem," see the section "Continuous symmetries: 'no $d=2$ crystal' theorem").

For more details, the reader is referred to Penrose and Onsager (1956), Yang (1962), Ruelle (1969), Hohenberg (1967), Gallavotti (1999), and Aizenman *et al.* (2004).

Appendix 1: The Physical Meaning of the Stability Conditions

It is useful to see what would happen if the conditions of stability and temperedness (see [14]) are violated. The analysis also illustrates some of the typical methods of statistical mechanics.

Coalescence Catastrophe due to Short-Distance Attraction

The simplest violation of the first condition in [14] occurs when the potential φ is smooth and negative at the origin.

Let $\delta > 0$ be so small that the potential at distances $\leq 2\delta$ is $\leq -b < 0$. Consider the canonical distribution with parameters β, N in a (cubic) box Ω of volume V. The probability P_{collapse} that all the N particles are located in a little sphere of radius δ around the center of the box (or around any prefixed point of the box) is estimated from below by remarking that

$$\Phi \leq -b\binom{N}{2} \sim -\frac{b}{2}N^2$$

so that

$$\begin{aligned} P_{\text{collapse}} &= \frac{\int_C \frac{\mathrm{d}p\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta(K(p)+\Phi(q))}}{\int \frac{\mathrm{d}p\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta(K(p)+\Phi(q))}} \\ &\geq \frac{\left(\frac{4\pi\sqrt{2m\beta^{-1}}^3}{3h^3}\right)^N \frac{\delta^{3N}}{N!}\mathrm{e}^{\beta b(1/2)N(N-1)}}{\int \frac{\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta\Phi(q)}} \end{aligned} \qquad [71]$$

The phase space is extremely small: nevertheless, such configurations are far more probable than the configurations which "look macroscopically correct," that is, configurations with particles more or less spaced by the average particle distance expected in a macroscopically homogeneous configuration, namely $(N/V)^{-1/3} = \rho^{-1/3}$. Their energy $\Phi(q)$ is of the order of uN for some u, so that their probability will be bounded above by

$$\begin{aligned} P_{\text{regular}} &\leq \frac{\int \frac{\mathrm{d}p\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta(K(p)+uN)}}{\int \frac{\mathrm{d}p\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta(K(p)+\Phi(q))}} \\ &= \frac{\frac{V^N\sqrt{2m\beta^{-1}}^3}{h^{3N}N!}\mathrm{e}^{-\beta uN}}{\int \frac{\mathrm{d}q}{h^{3N}N!}\mathrm{e}^{-\beta\Phi(q)}} \end{aligned} \qquad [72]$$

However, no matter how small δ is, the ratio $P_{\text{regular}}/P_{\text{collapse}}$ will approach 0 as $V \to \infty$, $N/V \to v^{-1}$; this occurs extremely rapidly because $e^{\beta b N^2/2}$ eventually dominates over $V^N \sim e^{N \log N}$.

Thus, it is far more probable to find the system in a microscopic volume of size δ rather than in a configuration in which the energy has some macroscopic value proportional to N. This catastrophe can be called an ultraviolet catastrophe (as it is due to the behavior at very short distances) and it causes the collapse of the particles into configurations concentrated in regions as small as we please as $V \to \infty$.

Coalescence Catastrophe due to Long-Range Attraction

It occurs when the potential is too attractive near ∞. For simplicity, suppose that the potential has a hard core, i.e., it is $+\infty$ for $r < r_0$, so that the above-discussed coalescence cannot occur and the system density bounded above by a certain quantity $\rho_{\text{cp}} < \infty$ (*close-packing density*).

The catastrophe occurs if $\varphi(q) \sim -g|q|^{-3+\varepsilon}$, $g, \varepsilon > 0$, for $|q|$ large. For instance, this is the case for matter interacting gravitationally; if k is the gravitational constant, m is the particle mass, then $g = km^2$ and $\varepsilon = 2$.

The probability P_{regular} of "regular configurations," where particles are at distances of order $\rho^{-1/3}$ from their close neighbors, is compared with the probability P_{collapse} of "catastrophic configurations," with the particles at distances r_0 from their close neighbors to form a configuration of density $\rho_{\text{cp}}/(1+\delta)^3$ almost in close packing (so that r_0 is equal to the hard-core radius times $1+\delta$). In the latter case, the system does not fill the available volume and leaves empty a region whose volume is a fraction $\sim((\rho_{\text{cp}} - \rho)/\rho_{\text{cp}})V$ of V. Further, it can be checked that the ratio $P_{\text{regular}}/P_{\text{collapse}}$ tends to 0 at a rate $O(\exp(g\frac{1}{2}N(\rho_{\text{cp}}(1+\delta)^{-3} - \rho)))$ if δ is small enough (and $\rho < \rho_{\text{cp}}$).

A system which is too attractive at infinity will not occupy the available volume but will stay confined in a close-packed configuration even in empty space.

This is important in the theory of stars: stars cannot be expected to obey "regular thermodynamics" and in particular will not "evaporate" because their particles interact via the gravitational force at large distances. Stars do not occupy the whole volume given to them (i.e., the universe); they do not collapse to a point only because the interaction has a strongly repulsive core (even when they are burnt out and the radiation pressure is no longer able to keep them at a reasonable size).

Evaporation Catastrophe

This is another *infrared catastrophe*, that is, a catastrophe due to the long-range structure of the interactions in the above subsection; it occurs when the potential is too repulsive at ∞, that is,

$$\varphi(q) \sim +g|q|^{-3+\varepsilon} \quad \text{as} \quad q \to \infty$$

so that the temperedness condition is again violated.

In addition, in this case, the system does not occupy the whole volume: it will generate a layer of particles sticking, in close-packed configuration, to the walls of the container. Therefore, if the density is lower than the close-packing density, $\rho < \rho_{\text{cp}}$, the system will leave a region around the center of the container Ω empty; and the volume of the empty region will still be of the order of the total volume of the box (i.e., its diameter will be a fraction of the box side L). The proof is completely analogous to the one of the previous case; except that now the configuration with lowest energy will be the one sticking to the wall and close packed there, rather than the one close packed at the center.

Also this catastrophe is important as it is realized in systems of charged particles bearing the same charge: the charges adhere to the boundary in close-packing configuration, and dispose themselves so that the electrostatic potential energy is minimal. Therefore, charges deposited on a metal will not occupy the whole volume: they will rather form a surface layer minimizing the potential energy (i.e., so that the Coulomb potential in the interior is constant). In general, charges in excess of neutrality do not behave thermodynamically: for instance, besides not occupying the whole volume given to them, they will not contribute normally to the specific heat.

Neutral systems of charges behave thermodynamically if they have hard cores, so that the ultraviolet catastrophe cannot occur or if they obey quantum-mechanical laws and consist of fermionic particles (plus possibly bosonic particles with charges of only one sign).

For more details, we refer the reader to Lieb and Lebowitz (1972) and Lieb and Thirring (2001).

Appendix 2: The Subadditivity Method

A simple consequence of the assumptions is that the exponential in (5.2) can be bounded above by $e^{\beta B N} \exp(-\frac{\beta}{2m}\sum_{i=1}^{N} P_i^2)$ so that

$$1 \le Z_{\text{gc}}(\beta, \lambda, V) \le \exp\left(V e^{\beta\lambda} e^{\beta B} \sqrt{2m\beta^{-1}}^{d}\right)$$

$$\Rightarrow 0 \le \frac{1}{V}\log Z_{\text{gc}}(\beta, \lambda, V) \le e^{\beta\lambda} e^{\beta B} \sqrt{2m\beta^{-1}}^{d} \quad [73]$$

Consider, for simplicity, the case of a hard-core interaction with finite range (cf. [14]). Consider a

sequence of boxes Ω_n with sides $2^n L_0$, where $L_0 > 0$ is arbitrarily fixed to be $> 2R$. The partition function $Z_{gc}(\beta, z)$ relative to the volume Ω_n is

$$Z_n = \sum_{N=0}^{\infty} \frac{z^N}{N!} \int_{\Omega_n} d\mathbf{Q} e^{-\beta \Phi(\mathbf{Q})}$$

because the integral over the $\boldsymbol{P}$ variables can be explicitly performed and included in z^N if z is defined as $z = e^{\beta\lambda}(2m\beta^{-1})^{d/2}$.

Then the box Ω_n contains 2^d boxes Ω_{n-1} for $n \geq 1$ and

$$1 \leq Z_n \leq Z_{n-1}^{2^d} \exp\left(\beta B 2d (L_{n-1}/R)^{d-1} 2^{2d}\right) \quad [74]$$

because the corridor of width $2R$ around the boundaries of the 2^d cubes Ω_{n-1} filling Ω_n has volume $2RL_{n-1}2^d$ and contains at most $(L_{n-1}/R)^{d-1}2^d$ particles, each of which interacts with at most 2^d other particles. Therefore,

$$\beta p_n \stackrel{\text{def}}{=} L_n^d \log Z_n \leq L_{n-1}^d \log Z_{n-1} + \beta B \gamma_d 2^{-n} (L_0/R)^{d-1}$$

for some $\gamma_d > 0$. Hence, $0 \leq \beta p_n \leq \beta p_{n-1} + \Gamma_d 2^{-n}$ for some $\Gamma_d > 0$ and p_n is bounded above and below uniformly in n. So, the limit [13] exists on the sequence $L_n = L_0 2^n$ and defines a function $\beta p_\infty(\beta, \lambda)$.

A box of arbitrary size L can be filled with about $(L/L_{\bar{n}})^d$ boxes of side $L_{\bar{n}}$ with $\bar{n}$ so large that, prefixed $\delta > 0$, $|p_\infty - p_n| < \delta$ for all $n \geq \bar{n}$. Likewise, a box of size L_n can be filled by about $(L_n/L)^d$ boxes of size L if n is large. The latter remarks lead us to conclude, by standard inequalities, that the limit in [13] exists and coincides with p_∞.

The subadditivity method just demonstrated for finite-range potentials with hard core can be extended to the potentials satisfying just stability and temperedness (cf. the section "Thermodynamic limit").

For more details, the reader is referred to Ruelle (1969) and Gallavotti (1999).

Appendix 3: An Infrared Inequality

The infrared inequalities stem from *Bogoliubov's inequality*. Consider as an example the problem of crystallization discussed in the section "Continuous symmetries: 'no $d = 2$ crystal' theorem". Let $\langle\cdot\rangle$ denote average over a canonical equilibrium state with Hamiltonian

$$H = \sum_{j=1}^{N} \frac{p_j^2}{2} + U(\mathbf{Q}) + \varepsilon W(\mathbf{Q})$$

with given temperature and density parameters $\beta, \rho, \rho = a^{-3}$. Let $\{X, Y\} = \sum_j (\partial_{p_j} X \partial_{q_j} Y - \partial_{q_j} X \partial_{p_j} Y)$ be the Poisson bracket. Integration by parts, with periodic boundary conditions, yields

$$\langle A^*\{C, H\}\rangle \equiv -\frac{\int A^*\{C, e^{-\beta H}\} d\boldsymbol{P} d\boldsymbol{Q}}{\beta Z_c(\beta, \rho, N)} \equiv -\beta^{-1}\langle\{A^*, C\}\rangle \quad [75]$$

as a general identity. The latter identity implies, for $A = \{C, H\}$, that

$$\langle\{H, C\}^*\{H, C\}\rangle = -\beta^{-1}\langle\{C, \{H, C^*\}\}\rangle \quad [76]$$

Hence, the Schwartz inequality $\langle A^* A\rangle\langle\{H, C\}^* \{H, C\}\rangle \geq |\langle\{A^*, C\}\rangle|^2$ combined with the two relations in [75], [76] yields Bogoliubov's inequality:

$$\langle A^* A\rangle \geq \beta^{-1} \frac{|\langle\{A^*, C\}\rangle|^2}{\langle\{C, \{C^*, H\}\}\rangle} \quad [77]$$

Let g, h be arbitrary complex (differentiable) functions and $\partial_j = \partial_{q_j}$

$$A(\mathbf{Q}) \stackrel{\text{def}}{=} \sum_{j=1}^{N} g(\boldsymbol{q}_j), \qquad C(\boldsymbol{P}, \mathbf{Q}) \stackrel{\text{def}}{=} \sum_{j=1}^{N} \boldsymbol{p}_j h(\boldsymbol{q}_j) \quad [78]$$

Then $H = \sum \frac{1}{2}\boldsymbol{p}_j^2 + \Phi(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_N)$, if

$$\Phi(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_N) = \frac{1}{2}\sum_{j \neq j'} \varphi(|\boldsymbol{q}_j - \boldsymbol{q}_{j'}|) + \varepsilon \sum_j W(\boldsymbol{q}_j)$$

so that, via algebra,

$$\{C, H\} \equiv \sum_j (h_j \partial_j \Phi - \boldsymbol{p}_j (\boldsymbol{p}_j \cdot \partial_j) h_j)$$

with $h_j \stackrel{\text{def}}{=} h(\boldsymbol{q}_j)$. If h is real valued, $\langle\{C, \{C^*, H\}\}\rangle$ becomes, again via algebra,

$$\left\langle \sum_{jj'} h_j h_{j'} \partial_j \cdot \partial_{j'} \Phi(\mathbf{Q}) \right\rangle + \left\langle \varepsilon \sum_j h_j^2 \Delta W(\boldsymbol{q}_j) + \frac{4}{\beta} \sum_j (\partial_j h_j)^2 \right\rangle$$

(integrals on $\boldsymbol{p}_j$ just replace $\boldsymbol{p}_j^2$ by $2\beta^{-1}$ and $\langle(\boldsymbol{p}_j)_i (\boldsymbol{p}_j)_{i'}\rangle = \beta^{-1}\delta_{i,i'}$). Therefore, the average $\langle\{C, \{C^*, H\}\}\rangle$ becomes

$$\left\langle \frac{1}{2}\sum_{jj'} (h_j - h_{j'})^2 \Delta\varphi(|\boldsymbol{q}_j - \boldsymbol{q}_{j'}|) + \varepsilon \sum_j h_j^2 \Delta W(\boldsymbol{q}_j) + 4\beta^{-1} \sum_j (\partial_j h_j)^2 \right\rangle \quad [79]$$

Choose $g(\boldsymbol{q}) \equiv e^{-i(\boldsymbol{\kappa}+K)\cdot\boldsymbol{q}}$, $h(\boldsymbol{q}) = \cos \boldsymbol{q} \cdot \boldsymbol{\kappa}$ and bound $(h_j - h_{j'})^2$ by $\boldsymbol{\kappa}^2(\boldsymbol{q}_j - \boldsymbol{q}_{j'})^2$, $(\partial_j h_j)^2$ by $\boldsymbol{\kappa}^2$ and

h_j^2 by 1. Hence [79] is bounded above by $ND(\boldsymbol{\kappa})$ with

$$D(\boldsymbol{\kappa}) \stackrel{\text{def}}{=} \left\langle \boldsymbol{\kappa}^2 \left(4\beta^{-1} + \frac{1}{2N} \sum_{j \neq j'} (\boldsymbol{q}_j - \boldsymbol{q}_{j'})^2 |\Delta\varphi(\boldsymbol{q}_j - \boldsymbol{q}_{j'})| \right) + \varepsilon \frac{1}{N} \sum_j |\Delta W(\boldsymbol{q}_j)| \right\rangle \quad [80]$$

This can be used to estimate the denominator in [77]. For the LHS remark that

$$\langle A^*, A \rangle = |\sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{\kappa}+\boldsymbol{K})}|^2$$

and

$$|\langle\{A^*, C\}\rangle|^2 = \left| \left\langle \sum_j h_j \partial g_j \right\rangle \right|^2 = |\boldsymbol{K} + \boldsymbol{\kappa}|^2 N^2 (\rho_\varepsilon(\boldsymbol{K}) + \rho_\varepsilon(\boldsymbol{K} + 2\boldsymbol{\kappa}))^2$$

hence [77] becomes, after multiplying both sides by the auxiliary function $\gamma(\boldsymbol{\kappa})$ (assumed even and vanishing for $|\boldsymbol{\kappa}| > \pi/a$) and summing over $\boldsymbol{\kappa}$,

$$D_1 \stackrel{\text{def}}{=} \frac{1}{N} \sum_{\boldsymbol{\kappa}} \gamma(\boldsymbol{\kappa}) \left\langle \frac{1}{N} |\sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}(\boldsymbol{K}+\boldsymbol{\kappa})\cdot\boldsymbol{q}_j}|^2 \right\rangle \geq \frac{1}{N} \sum_{\boldsymbol{\kappa}} \gamma(\boldsymbol{\kappa}) \times \frac{|\boldsymbol{K}|^2}{4\beta} \frac{(\rho_\varepsilon(\boldsymbol{K}) + \rho_\varepsilon(\boldsymbol{K} + 2\boldsymbol{\kappa}))^2}{D(\boldsymbol{\kappa})} \quad [81]$$

To apply [77] the averages in [80], [81] have to be bounded above: this is a technical point that is discussed here, as it illustrates a general method of using the results on the thermodynamic limits and their convexity properties to obtain estimates.

Note that $\langle (1/N) \sum_{\boldsymbol{k}} \gamma(\boldsymbol{k}) \mathrm{d}^d\boldsymbol{k} | \sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{q}_j}|^2 \rangle$ is identically $\widetilde{\varphi}(0) + (2/N)\langle \sum_{j<j'} \widetilde{\varphi}(\boldsymbol{q}_j - \boldsymbol{q}_{j'}) \rangle$ with $\widetilde{\varphi}(\boldsymbol{q}) \stackrel{\text{def}}{=} (1/N) \sum_{\boldsymbol{\kappa}} \gamma(\boldsymbol{\kappa}) \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{q}}$.

Let $\varphi_{\lambda,\zeta}(\boldsymbol{q}) \stackrel{\text{def}}{=} \varphi(\boldsymbol{q}) + \lambda\boldsymbol{q}^2 |\Delta\varphi(\boldsymbol{q})| + \eta\widetilde{\varphi}(\boldsymbol{q})$ and let $F_V(\lambda, \eta, \zeta) \stackrel{\text{def}}{=} (1/N) \log Z^{\mathrm{c}}(\lambda, \eta, \zeta)$ with Z^{c} the partition function in the volume Ω computed with energy $U' = \sum_{jj'} \varphi_{\lambda,\zeta}(\boldsymbol{q}_j - \boldsymbol{q}_{j'}) + \varepsilon \sum_j W(\boldsymbol{q}_j) + \eta\varepsilon \sum |\Delta W(\boldsymbol{q}_j)|$. Then $F_V(\lambda, \eta, \zeta)$ is convex in λ, η and it is uniformly bounded above and below if $|\eta|, |\varepsilon|, |\zeta| \leq 1$ (say) and $|\lambda| \leq \lambda_0$: here $\lambda_0 > 0$ exists if $\boldsymbol{r}^2 |\Delta\varphi(\boldsymbol{r})|$ satisfies the assumption set at the beginning of the section "Continuous symmetries: 'no $d = 2$ crystal' theorem" and the density is smaller than a close packing (this is because the potential U' will still satisfy conditions similar to [14] uniformly in $|\varepsilon|, |\eta| < 1$ and $|\lambda|$ small enough).

Convexity and boundedness above and below in an interval imply bounds on the derivatives in the interior points, in this case on the derivatives of F_V with respect to λ, η, ζ at 0. The latter are identical to the averages in [80], [81]. In this way, the constants B_1, B_2, B_0 such that $D(\boldsymbol{\kappa}) \leq \boldsymbol{\kappa}^2 B_1 + \varepsilon B_2$ and $B_0 > D_1$ are found.

For more details, the reader is referred to Mermin (1968).

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Introductory Article: Functional Analysis

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Introduction

Functional analysis is concerned with the study of functions and function spaces, combining techniques borrowed from classical analysis with algebraic techniques. Modern functional analysis developed around the problem of solving equations with solutions given by functions. After the differential and partial differential equations, which were studied in the eighteenth century, came the integral equations and other types of functional equations investigated in the nineteenth century, at the end of which arose the need to develop a new analysis, with functions of an infinite number of variables instead of the usual functions. In 1887, Volterra, inspired by the calculus of variations, suggested a new infinitesimal calculus where usual functions are replaced by functionals, that is, by maps from a function space to $\mathbb{R}$ or $\mathbb{C}$, but he and his followers were still missing some algebraic and topological tools to be developed later. Modern analysis was born with the development of an "algebra of the infinite" closely related to classical linear algebra which by 1890 had (up to the concept of duality, which was developed later) settled on firm ground. Strongly inspired by algebraic methods, Fredholm's work at the turn of the nineteenth century, in which emerged the concept of kernel of an operator, became a founding stone for the modern theory of integral equations. Hilbert developed further Fredholm's methods for symmetric kernels, exploiting analogies with the theory of real quadratic forms and thereby making clear the importance of the notion of square-integrable functions. With Hilbert's *Grundzüge einer allgemeinen Theorie der Integralgleichung*, a further step was made from the "algebra of the infinite" to the "geometry of the infinite." The contribution of Fréchet, who introduced the abstract notion of a space endowed with a distance, made it possible to transfer Euclidean geometry to the framework of what have since then been called Hilbert spaces, a basic concept in mathematics and quantum physics.

The usefulness of functional analysis in the study of quantum systems became clear in the 1950s when Kato proved the self-adjointness of atomic Hamiltonians, and Garding and Wightman formulated axioms for quantum field theory. Ever since functional analysis lies at the very heart of many approaches to quantum field theory. Applications of functional analysis stretch out to many branches of mathematics, among which are numerical

analysis, global analysis, the theory of pseudodifferential operators, differential geometry, operator algebras, noncommutative geometry, etc.

Topological Vector Spaces

Most topological spaces one comes across in practice are metric spaces. A metric on a topological space E is a map $d: E \times E \to [0, +\infty[$ which is symmetric, such that $d(u,v) = 0 \Leftrightarrow u = v$ and which verifies the triangle inequality $d(u,w) \leq d(u,v) + d(v,w)$ for all vectors u, v, w. A topological space E is metrizable if there is a metric d on E compatible with the topology on E, in which case the balls with radius $1/n$ centered at any point $x \in E$ form a local base at x – that is, a collection of neighborhoods of x such that every neighborhood of x contains a member of this collection. A sequence (u_n) in E then converges to $u \in E$ if and only if $d(u_n, u)$ converges to 0.

The Banach fixed-point theorem on a complete metric space (E, d) is a useful tool in nonlinear functional analysis: it states that *a (strict) contraction on E, that is, a map $T: E \to E$ such that $d(Tu, Tv) \leq k(u,v)$ for all $u \neq v \in E$ and fixed $0 < k < 1$, has a unique fixed point $Tu_0 = u_0$*. In particular, it provides local existence and uniqueness of solutions of differential equations $dy/dt = F(y,t)$ with initial condition $y(0) = y_0$, where F is Lipschitz continuous.

Linear functional analysis starts from topological vector spaces, that is, vector spaces equipped with a topology for which the operations are continuous. A topological vector space equipped with a local base whose members are convex is said to be locally convex. Examples of locally convex spaces are normed linear spaces, namely vector spaces equipped with a norm, a concept that first arose in the work of Fréchet. A seminorm on a vector space V is a map $\rho: V \to [0,\infty[$ which obeys the triangle identity $\rho(u+v) \leq \rho(u) + \rho(v)$ for any vectors u, v and such that $\rho(\lambda u) = |\lambda| \rho(u)$ for any scalar λ and any vector u; if $\rho(u) = 0 \Rightarrow u = 0$, it is a norm, often denoted by $\| \cdot \|$. A norm on a vector space E gives rise to a translation-invariant distance function $d(u,v) = \|u - v\|$ making it a metric space.

Historically, one of the first examples of normed spaces is the space $C([0,1])$ investigated by Riesz of (real- or complex-valued) continuous functions on the interval $[0,1]$ equipped with the supremium norm $\|f\|_\infty := \sup_{x \in [0,1]} |f(x)|$. In the 1920s, the general definition of Banach space arose in connection with the works of Hahn and Banach. A normed linear space is a Banach space if it is complete as a metric space for the induced metric, $C([0,1])$ being a prototype of a Banach space. More generally, for any non-negative integer k, the space $C^k([0,1])$ of functions on $[0,1]$ of class C^k equipped with the norm $\|f\|_k = \sum_{i=0}^{k} \|f^{(i)}\|_\infty$ expressed in terms of a finite number of seminorms $\|f^{(i)}\|_\infty = \sup_{x \in [0,1]} |f^{(i)}(x)|, i = 0, \ldots, k$, is also a Banach space.

The space $C^\infty([0,1])$ of smooth functions on the interval $[0,1]$ is not anymore a Banach space since its topology is described by a countable family of seminorms $\|f\|_k$ with k varying in the positive integers. The metric

$$d(f,g) = \sum_{k=1}^{\infty} 2^{-k} \frac{\|f-g\|_k}{1 + \|f-g\|_k}$$

turns it into a Fréchet space, that is, a locally convex complete metric space. The space $\mathcal{S}(\mathbb{R}^n)$ of rapidly decreasing functions, which are smooth functions f on $\mathbb{R}^n$ for which

$$\|f\|_{\alpha,\beta} := \sup_{x \in \mathbb{R}^n} |x^\alpha D_x^\beta f(x)|$$

is finite for any multiindices α and β, is also a Fréchet space with the topology given by the seminorms $\| \cdot \|_{\alpha,\beta}$. Further examples of Fréchet spaces are the space $C_0^\infty(K)$ of smooth functions with support in a fixed compact subset $K \subset \mathbb{R}^n$ equipped with the countable family of seminorms

$$\|D^\alpha f\|_{\infty,K} = \sup_{x \in K} |D_x^\alpha f(x)|, \quad \alpha \in \mathbb{N}_0^n$$

and the space $C^\infty(M,E)$ of smooth sections of a vector bundle E over a closed manifold M equipped with a similar countable family of seminorms. Given an open subset $\Omega = \cup_{p \in \mathbb{N}} K_p$ with $K_p, p \in \mathbb{N}$ compact subsets of $\mathbb{R}^n$, the space $\mathcal{D}(\Omega) = \cup_{p \in \mathbb{N}} C_0^\infty(K_p)$ equipped with the inductive limit topology – for which a sequence (f_n) in $\mathcal{D}(\Omega)$ converges to $f \in \mathcal{D}(\Omega)$ if each f_n has support in some fixed compact subset K and $(D^\alpha f_n)$ converges uniformly to $D^\alpha f$ on K for each mutilindex α – is a locally convex space.

Among Banach spaces are Hilbert spaces which have properties very similar to those of finite-dimensional spaces and are historically the first type of infinite-dimensional space to appear with the works of Hilbert at the beginning of the twentieth century. A Hilbert space is a Banach space equipped with a norm $\| \cdot \|$ that derives from an inner product, that is, $\|u\|^2 = \langle u, u \rangle$ with $\langle \cdot, \cdot \rangle$ a positive-definite bilinear (or sesquilinear according to whether the base space is real or complex) form. Hilbert spaces are fundamental building blocks in quantum mechanics; using (closed) tensor products, from a Hilbert space H one builds the Fock space $\mathcal{F}(H) = \sum_{k=0}^{\infty} \otimes^k H$ and from there the bosonic Fock space $\mathcal{F}(H) = \sum_{k=0}^{\infty} \otimes_s^k H$ (where $\otimes_s$ stands for the (closed) symmetrized tensor product) as well

as the fermionic Fock space $\mathcal{F}(H) = \sum_{k=0}^{\infty} \Lambda^k H$ (where Λ^k stands for the antisymmetrized (closed) tensor product).

A prototype of Hilbert space is the space $l_2(\mathbb{Z})$ of complex-valued sequences $(u_n)_{n\in\mathbb{Z}}$ such that $\sum_{n\in\mathbb{Z}} |u_n|^2$ is finite, which is already implicit in Hilbert's Grundzügen. Shortly afterwords, Riesz and Fischer, with the help of the integration tool introduced by Lebesgue, showed that the space $L^2(]0,1[)$ (first introduced by Riesz) of square-summable functions on the interval $]0,1[$, that is, functions f such that

$$\|f\|_{L^2} = \left(\int_0^1 |f(x)|^2 \, dx\right)^{1/2}$$

is finite, provides an example of Hilbert space. These were then further generalized to spaces $L^p(]0,1[)$ of p-summable $(1 \leq p < \infty)$ functionals on $]0,1[$ (i.e., functions f such that

$$\|f\|_{L^p} = \left(\int_0^1 |f(x)|^p \, dx\right)^{1/p}$$

is finite), which are not Hilbert unless $p=2$ but which provide further examples of Banach spaces, the space $L^\infty(]0,1[)$ of functions on $]0,1[$ bounded almost everywhere with respect to the Lebesgue measure, offering yet another example of Banach space.

In 1936, Sobolev gave a generalization of the notion of function and their derivatives through integration by parts, which led to the so-called Sobolev spaces $W^{k,p}(]0,1[)$ of functions $f \in L^p(]0,1[)$ with derivatives up to order k lying in $L^p(]0,1[)$, obtained as the closure of $C^\infty(]0,1[)$ for the norm

$$f \mapsto \|f\|_{W^{k,p}} = \left(\sum_{j=1}^{k} \|\partial^j f\|_{L^p}^p\right)^{1/p}$$

(for $p=2$, $W^{k,p}(]0,1[)$ is a Hilbert space often denoted by $H^k(]0,1[)$. They differ from the Sobolev spaces $W_0^{k,p}(]0,1[)$, which correspond to the closure of the set $\mathcal{D}(]0,1[)$ for the norm $f \mapsto \|f\|_{W^{k,p}}$; for example, an element $u \in W^{1,p}(]0,1[)$ lies in $W_0^{1,p}(]0,1[)$ if and only if it vanishes at 0 and 1, that is, if and only if it satisfies Dirichlet-type boundary conditions on the boundary of the interval. Similarly, one defines Sobolev spaces $W_0^{k,p}(\mathbb{R}) = W^{k,p}(\mathbb{R})$ on $\mathbb{R}$, Sobolev spaces $W^{k,p}(\Omega)$ and $W_0^{k,p}(\Omega)$ on open subsets $\Omega \subset \mathbb{R}^n$ and using a partition of unity on a closed manifold M, Sobolev spaces $H^k(M,E) = W^{k,2}(M,E)$ of sections of vector bundles E over M. Using the Fourier transform (discussed later), one can drop the assumption that k be an integer and extend the notion of Sobolev space to define $W^{s,p}(\Omega)$ and $H^s(M,E)$ with s any real number.

Sobolev spaces arise in many areas of mathematics; one central example in probability theory is the Cameron–Martin space $H^1([0,t])$ embedded in the Wiener space $C([0,t])$. This embedding is a particular case of more general Sobolev embedding theorems, which embed (possibly continuously, sometimes even compactly (the notion of compact operator is discussed in a later section)) $W^{k,p}$-Sobolev spaces in L^q-spaces with $q > p$ such as the continuous inclusion $W^{k,p}(\mathbb{R}^n) \subset L^q(\mathbb{R}^n)$ with $1/q = 1/p - k/n$, or in C^l-spaces with $l \leq k$ such as, for a bounded open and regular enough subset Ω of $\mathbb{R}^n$ and for any $s \geq l + n/p$ with $p > n$, the continuous inclusion $W^{s,p}(\Omega) \subset C^l(\bar{\Omega})$ (the set of functions in $C^l(\Omega)$ such that $D^\alpha u$ can be continuously extended to the closure $\bar{\Omega}$ for all $|\alpha| \leq l$). Sobolev embeddings have important applications for the regularity of solutions of partial differential equations, when showing that weak solutions one constructs are in fact smooth. In particular, on an n-dimensional closed manifold M for $s > l + n/2$, the Sobolev space $H^s(M,E)$ can be continuously embedded in the space $C^l(M,E)$ of sections of E of class C^l, which in particular implies that the solutions of a hypoelliptic partial differential equation $Au = v$ with $v \in L^2(M,E)$ are smooth, as for example in the case of solutions of the Seiberg–Witten equations.

Duality

The concept of duality (in a topological sense) was initiated at the beginning of the twentieth century by Hadamard, who was looking for continuous linear functionals on the Banach space $C(I)$ of continuous functions on a compact interval I equipped with a uniform topology. It is implicit in Hilbert's theory and plays a central part in Riesz' work, who managed to express such continuous functionals as Stieltjes integrals, one of the starting points for the modern theory of integration.

The topological dual of a topological vector space E is the space E^* of continuous linear forms on E which, when E is a normed space, can be equipped with the dual norm $\|L\|_{E^*} = \sup_{u\in E, \|u\|\leq 1} |L(u)|$.

Dual spaces often provide a receptacle for singular objects; any of the functions $f \in L^p(\mathbb{R}^n)(p \geq 1)$ and the delta-function at point $x \in \mathbb{R}^n$, $\delta_x : f \mapsto f(x)$, all lie in the space $\mathcal{S}'(\mathbb{R}^n)$ dual to $\mathcal{S}(\mathbb{R}^n)$ of tempered distributions on $\mathbb{R}^n$, which is itself contained in the space $\mathcal{D}'(\mathbb{R}^n)$ of distributions dual to $\mathcal{D}(\mathbb{R}^n)$. Furthermore, the topological dual E^* of a nuclear space E contains the support of a probability

measure with characteristic function (see the next section) given by a continuous positive-definite function on E. Among nuclear spaces are projective limits $E = \cap_{p\in\mathbb{N}} H_p$ (a sequence $(u_n) \in E$ converges to $u \in E$ whenever it converges to u in each H_p) of countably many nested Hilbert spaces $\cdots \subset H_p \subset H_{p-1} \subset \cdots \subset H_0$ such that the embedding $H_p \subset H_{p-1}$ is a trace-class operator (see the section "Operator algebras"). If H_p is the closure of E for the norm $\|\cdot\|_p$, the topological dual E' of E for the norm $\|\cdot\|_0$ is an inductive limit $E' = \cup_{p\in\mathbb{N}_0} H_{-p}$, where H_{-p} are the dual (with respect to $\|\cdot\|_0$) Hilbert spaces with norm $\|\cdot\|_{-p}$ (a sequence $(u_n) \in E'$ converges to $u \in E'$ whenever it lies in some H_{-p} and converges to u for the topology of H_{-p}) and we have

$$E \subset \cdots \subset H_p \subset H_{p-1} \subset \cdots \subset H_0 = H_0' \subset H_{-1} \subset \cdots \subset H_{-p} \subset \cdots \subset E'$$

As a result of the theory of elliptic operators on a closed manifold, the Fréchet space $C^\infty(M,E)$ of smooth sections of a vector bundle over a closed manifold M is nuclear as the inductive limit of countably many Sobolev spaces $H^p(M,E)$ with L^2-dual given by the projective limit of countably many Sobolev spaces $H^{-p}(M,E)$.

The existence of nontrivial continuous linear forms on a normed linear space E is ensured by the Hahn–Banach theorem, which asserts that *for any closed linear subspace F of E, there is a nonvanishing continuous linear form that vanishes on F*. When the space is a Hilbert space $(H,\langle\cdot,\cdot\rangle_H)$, it follows from the Riesz–Fréchet theorem that any continuous linear form L on H is represented in a unique way by a vector $v \in H$ such that $L(u) = \langle v,u\rangle_H$ for all $u \in H$, thus relating the dual pairing on the left with the Hilbert inner product on the right and identifying the topological dual H^* with H.

The strong topology induced by the norm $\|\cdot\|$ on a normed vector space E – that is, the topology in which a sequence (u_n) converges to u whenever $\|u_n - u\| \to 0$ – is too refined to have compact sets when E is infinite dimensional since the compactness of the unit ball in E for the strong topology characterizes finite-dimensional spaces. Since compact sets are useful for existence theorems, one is inclined to weaken the topology: the weak topology on E – which coincides with the strong topology when E is finite dimensional and for which a sequence (u_n) converges to u if and only if $L(u_n) \to L(u)\ \forall L \in E^*$ – has compact unit ball if and only if E is reflexive or, in other words, if E can be canonically identified with its double dual $(E^*)^*$. For $1 < p < \infty$, given an open subset $\Omega \subset \mathbb{R}^n$, the topological dual of $L^p(\Omega)$ can be identified via the Riesz representation with $L^{p^*}(\Omega)$ with p^* conjugate to p, that is, $1/p + 1/p^* = 1$ and $L^p(\Omega)$ is reflexive, whereas the topological duals of $W^{s,p}(\Omega)$ and $W_0^{s,p}(\Omega)$ both coincide with $W_0^{-s,p^*}(\Omega)$ so that only $W_0^{s,p}(\Omega)$ is reflexive. Neither $L^1(\Omega)$ nor its topological dual $L^\infty(\Omega)$ is reflexive since $L^1(\Omega)$ is strictly contained in the topological dual of $L^\infty(\Omega)$ for there are continuous linear forms L on $L^\infty(\Omega)$ that are not of the form

$$L(u) = \int_\Omega uv \ \forall u \in L^\infty(\Omega) \quad \text{with } v \in L^1(\Omega)$$

Similarly, the topological dual E^* of a normed linear space E can be equipped with the topology induced by the dual norm $\|\cdot\|_{E^*}$ and the the weak $*$-topology, namely the weakest one for which the maps $L \mapsto L(u), u \in E$, are continuous, and the unit ball in E^* is indeed compact for this topology (Banach–Alaoglu theorem).

Duality does not always preserve separability – a topological vector space is separable if it has a countable dense subspace – since $L^\infty(\Omega)$, which is not separable, is the topological dual of $L^1(\Omega)$, which is separable. However, as a consequence of the Hahn–Banach theorem, if the topological dual of a Banach space is separable then so is the original space and one has equivalence when adding the reflexivity assumption; a Banach space is reflexive and separable whenever its topological dual is. For $1 \le p < \infty$, $L^p(\Omega)$ and $W_0^{s,p}(\Omega)$ are separable and moreover reflexive if $p \neq 1$.

Fourier Transform

In the middle of the eighteenth century, oscillations of a vibrating string were interpreted by Bernouilli as a limit case for the oscillation of n-point masses when n tends the infinity, and Bernouilli introduced the novel idea of the superposition principle by which the general oscillation of the string should decompose in a superposition of "proper oscillations." This point of view triggered off a discussion as to whether or not an arbitrary function can be expanded as a trigonometric series. Other examples of expansions in "orthogonal functions" (this terminology actually only appears with Hilbert) had been found in the mean time in relation to oscillation problems and investigations on heat theory, but it was only in the nineteenth century, with the works of Fourier and Dirichlet, that the superposition problem was solved.

Separable Hilbert spaces can be equipped with a countable orthonormal system $\{e_n\}_{n\in\mathbb{Z}}$ ($\langle e_n, e_m\rangle_H = \delta_{mn}$ with $\langle\cdot,\cdot\rangle_H$ the scalar product on H) which is

complete, that is, any vector $u \in H$ can be expanded in this system in a unique way $u = \sum_{n\in\mathbb{Z}} \hat{u}_n e_n$ with Fourier coefficients $\hat{u}_n = \langle u, e_n\rangle$. The latter obey Parseval's relation $\sum_{n\in\mathbb{Z}} |\hat{u}_n|^2 = \|u\|^2$ (where $\|\cdot\|$ is the norm associated with $\langle\cdot,\cdot\rangle$), and the Fourier transform $u \mapsto (\hat{u}(n))_{n\in\mathbb{Z}}$ gives rise to an isometric isomorphism between the separable Hilbert space H and the Hilbert space $l^2(\mathbb{Z})$ of square-summable sequences of complex numbers. In particular, the space $L^2(S^1)$ of L^2-functions on the unit circle $S^1 = \mathbb{R}/\mathbb{Z}$ with its usual Haar measure dt is separable with complete orthonormal system $t \mapsto e_n(t) = e^{2i\pi nt}, n \in \mathbb{Z}$ and the Fourier transform

$$u \mapsto \left(t \mapsto \hat{u}(n) = \int_0^1 e^{-2i\pi nt} u(t)\, dt\right)_{n\in\mathbb{Z}}$$

identifies it with the space $l^2(\mathbb{Z})$. Under this identification, the Hilbert subspace $l^2(\mathbb{N})$ obtained as the range in $l^2(\mathbb{Z})$ of the projection $p_+ : (u)_{n\in\mathbb{Z}} \mapsto (u_n)_{n\in\mathbb{N}}$ corresponds to the Hardy space $\mathcal{H}^2(S^1)$.

The Fourier transform extends to the space $\mathcal{S}(\mathbb{R}^n)$, sending a function $f \in \mathcal{S}(\mathbb{R}^n)$ to the map

$$\xi \mapsto \hat{f}(\xi) = \frac{1}{\sqrt{(2\pi)^n}} \int_{\mathbb{R}^n} e^{-i\xi\cdot x} f(x)\, dx$$

and maps $\mathcal{S}(\mathbb{R}^n)$ onto itself linearly and continuously with continuous inverse $f \mapsto \hat{f}(-\xi)$. When $n = 1$, the Poisson formula relates $f \in \mathcal{S}(\mathbb{R})$ with its Fourier transform $\hat{f}$ by $\sum_{n=-\infty}^{\infty} f(2\pi n) = \sum_{n=-\infty}^{\infty} \hat{f}(n)$.

Since Fourier transformation turns (up to a constant multiplicative factor) differentiation D_ξ^α for a multiindex $\alpha = (\alpha_1, \ldots, \alpha_n)$ into multiplication by $\xi^\alpha = \xi_1^{\alpha_1} \cdots \xi_n^{\alpha_n}$, it can be used to define $W^{s,p}$-Sobolev spaces with s a real number as the space of L^p-functions with finite Sobolev norms $\|u\|_{W^{s,p}} = (\int |(1 + |\xi|)^s \hat{u}(\xi)|^p)^{1/p}$ (which coincide with the ones defined previously when $s = k$ is a non-negative integer).

Fourier transforms are also used to describe a linear pseudodifferential operator A (see next two sections where the notions of bounded and unbounded linear operator are discussed) of order a acting on smooth functions on an open subset U of $\mathbb{R}^n$ in terms of its symbol σ_A – a smooth map σ on $U \times \mathbb{R}^n$ with compact support in x such that for any multi-indices $\alpha, \beta \in \mathbb{N}_0^n$, there is a constant $C_{\alpha,\beta}$ with

$$|D_x^\alpha D_\xi^\beta \sigma(x,\xi) \le C_{\alpha,\beta}(1 + |\xi|)^{a-|\beta|}$$

for any $\xi \in \mathbb{R}^n$ – by

$$(Af)(x) = \frac{1}{\sqrt{(2\pi)^n}} \int_{\mathbb{R}^n} e^{-ix\cdot\xi} \sigma_A(x,\xi) \hat{f}(\xi)\, d\xi$$

Fourier transform maps a Gaussian function $x \mapsto e^{-(1/2)\lambda|x|^2}$ on $\mathbb{R}^n$, where λ is a nonzero scalar, to another Gaussian function $\xi \mapsto e^{-(1/2)\lambda^{-1}|\xi|^2}$ (up to a nonzero multiplicative factor), a starting point for T-duality in string theory. More generally, the characteristic function

$$\hat{\mu}(\xi) := \int_H e^{i\langle x,\xi\rangle_H} \mu(dx)$$

of a Gaussian probability measure μ with covariance C on a Hilbert space H is the function $\xi \mapsto e^{-(1/2)\langle \xi, C\xi\rangle_H}$. Such probability measures typically arise in Euclidean quantum field theory; in axiomatic quantum field theory, the analyticity properties of n-point functions can be derived from the Wightman axioms using Fourier transforms. Thus, Fourier transformation underlies many different aspects of quantum field theory.

Fredholm operators

A complex-valued continuous function K on $[0,1] \times [0,1]$ gives rise to an integral operator

$$A : f \to \int_0^1 K(x,y) f(y)\, dy$$

on complex-valued continuous functions on $[0,1]$ (equipped with the supremum norm $\|\cdot\|_\infty$) with the following upper bound property:

$$\|Af\|_\infty \le \mathrm{Sup}_{[0,1]\times[0,1]} |K(x,y)|\, \|f\|_\infty$$

In other words, A is a bounded linear operator with norm bounded from above by $\sup_{[0,1]\times[0,1]} |K(x,y)|$; a linear operator $A : E \to F$ from a normed linear space $(E, \|\cdot\|_E)$ to a normed linear space $(F, \|\cdot\|_F)$ is bounded (or continuous) if and only if its (operator) norm $|||A||| := \sup_{\|u\|_E \le 1} \|Au\|_F$ is bounded.

An integral operator

$$A : f \to \int_0^1 K(x,y) f(y)\, dy$$

defined by a continuous kernel K is, moreover, compact; a compact operator is a bounded operator of normed spaces that maps bounded sets to a precompact sets, that is, to sets whose closure is compact. Other examples of compact operators on normed spaces are finite-rank operators, operators with finite-dimensional range. In fact, any compact operator on a separable Hilbert space can be approximated in the topology induced by the operator norm $|||\cdot|||$ by a sequence of finite-rank operators.

Inspired by the work of Volterra, who, in the case of the integral operator defined above, produced

continuous solutions $\phi = (I - A)^{-1} f$ of the equation $f = (I - A)\phi$ for $f \in C([0,1])$, Fredholm in 1900 (*Sur une classe d'équations fonctionnelles*) studied the equation $f = (I - \lambda A)\phi$, introducing a complex parameter λ. He proved what is since then called the Fredholm alternative, which states that either the equation $f = (I - \lambda A)\phi$ has a unique solution for every $f \in C([0,1])$ or the corresponding homogeneous equation $(I - \lambda A)\phi = 0$ has nontrivial solutions. In modern language, it means that the resolvent $R(A, \mu) = (A - \mu I)^{-1}$ of a compact linear operator A is surjective if and only if it is injective. The Fredholm alternative is a powerful tool to solve partial differential equations among which the Dirichlet problem, the solutions of which are harmonic functions u (i.e., $\Delta u = 0$, where $\Delta = -\sum_{i=1}^{n} \partial^2 u / \partial x_i^2$) on some domain $\Omega \in \mathbb{R}^n$ with Dirichlet boundary conditions $u_{|\partial\Omega} = f$, where f is a continuous function on the boundary $\partial\Omega$. The Dirichlet problem has geometric applications, in particular to the nonlinear Plateau problem, which minimizes the area of a surface in $\mathbb{R}^d$ with given boundary curves and which reduces to a (linear) Dirichlet problem.

The operator $B = I - A$ built from the compact operator A is a particular Fredholm operator, namely a bounded linear operator $B : E \to F$ which is invertible "up to compact operators," that is, such that there is a bounded linear operator $C : F \to E$ with both $BC - I_F$ and $CB - I_E$ compact. A Fredholm operator B has a finite-dimensional kernel $\mathrm{Ker}\, B$ and when $(E, \langle \cdot, \cdot \rangle_E)$ and $(F, \langle \cdot, \cdot \rangle_F)$ are Hilbert spaces its cokernel $\mathrm{Ker}\, B^*$, where B^* is the adjoint of B defined by

$$\langle Bu, v \rangle_F = \langle u, B^* v \rangle_E \quad \forall u \in E, \forall v \in F$$

is also finite dimensional, so that it has a well-defined index $\mathrm{ind}(B) = \dim(\mathrm{Ker}\, B) - \dim(\mathrm{Ker}\, B^*)$, a starting point for index theory. Töplitz operators T_ϕ, where ϕ is a continuous function on the unit circle S^1, provide first examples of Fredholm operators; they act on the Hardy space $\mathcal{H}^2(S^1)$ by

$$T_{e_{-n}} \left(\sum_{m \geq 0} a_m e_m \right) = \sum_{m \geq 0} a_{m+n} e_m$$

under the identification $\mathcal{H}^2(S^1) \simeq l^2(\mathbb{N}) \subset l^2(\mathbb{Z})$, with $l^2(\mathbb{Z})$ equipped with the canonical complete orthonormal basis $(e_n, n \in \mathbb{Z})$. The Fredholm index $\mathrm{ind}(T_{e_{-n}})$ is exactly the integer n so that the index of its adjoint is $-n$, as a consequence of which the index map from Fredholm operators to integers is onto.

One-Parameter (Semi) groups

Unlike in the finite-dimensional situation, a linear operator $A : E \to F$ between two normed linear spaces $(E, \| \cdot \|_E)$ and $(F, \| \cdot \|_F)$ is not expected to be bounded. Unbounded operators arise in partial differential equations that involve differential operators such as the Laplacian Δ on an open subset $\Omega \subset \mathbb{R}^n$. The following equations provide fundamental examples of partial differential equations which arose over time from the study of various problems in mathematical physics with the works of Poisson, Fourier, and Cauchy:

$$\Delta u = 0 \quad \text{Laplace equation}$$

$$\frac{\partial^2 t}{\partial t^2} + \Delta u = 0 \quad \text{wave equation}$$

$$\frac{\partial u}{\partial t} + \Delta u = 0 \quad \text{heat equation}$$

and later the Schrödinger equation in quantum mechanics:

$$\mathrm{i} \frac{\partial u}{\partial t} = \Delta u$$

where t is a time parameter.

An unbounded linear operator on an infinite-dimensional normed space is usually defined on a domain $D(A)$ which is strictly contained in E. The Laplacian Δ is defined on the dense domain $D(A) = H^2(\mathbb{R}^n)$ in $L^2(\mathbb{R}^n)$; it defines a bounded operator from $H^2(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$ but does not extend to a bounded operator on $L^2(\mathbb{R}^n)$. Like this operator, most unbounded operators $A : E \to F$ one comes across have dense domain $D(A)$ in E and are closed, that is, their graph $\{(u, Au), u \in D(A)\}$ is closed as a subset of the normed linear space $E \times F$. When not actually closed, they can be closable, that is, they can have a closed extension called the closure of the operator. By the closed-graph theorem, when E and F are Banach spaces, a linear operator $A : E \to F$ is continuous whenever its graph is closed, as a consequence of which a closed linear operator $A : E \to F$ defined on a dense domain is bounded provided its domain coincides with the whole space.

For a closed operator $A : E \to F$ with dense domain $D(A)$, when E and F are Hilbert spaces equipped with inner products $\langle \cdot, \cdot \rangle_E$ and $\langle \cdot, \cdot \rangle_F$, the adjoint A^* of A is defined on its domain $D(A^*)$ by

$$\langle Au, v \rangle_F = \langle u, A^* v \rangle_E \quad \forall (u, v) \in D(A) \times D(A^*)$$

A self-adjoint operator A with domain $D(A)$ is one for which $D(A) = D(A^*)$ and $A = A^*$; the Laplacian Δ on $\mathbb{R}^n$ is self-adjoint on the Sobolev space $H^2(\mathbb{R}^n)$ but it is only essentially self-adjoint on the dense domain $\mathcal{D}(\mathbb{R}^n)$, the latter meaning that its closure is self-adjoint.

Unbounded self-adjoint operators can arise as generators of one-parameter semigroups of bounded

operators. A one-parameter family of bounded operators $T_t, t \geq 0$ ($T_t, t \in \mathbb{R}$) on a Hilbert space H is a semigroup (resp. group) if $T_s T_t = T_{t+s}$ $\forall t, s \geq 0$ (resp. $\forall t, s \in \mathbb{R}$) and it is strongly continuous (or simply continuous) if $\lim_{t \to t_0} T_t u = T_{t_0} u$ at any $t_0 \geq 0$ (resp. $t_0 \in \mathbb{R}$) and for any $u \in H$.

Stones' theorem sets up a one-to-one correspondence between continuous one-parameter unitary ($U_t^* U_t = U_t U_t^* = I$) groups $U_t, t \in \mathbb{R}$ on a Hilbert space such that $U_0 = \mathrm{Id}$ and self-adjoint operators A obtained as infinitesimal generators, that is, as the strong limit

$$Au = \lim_{t \to 0} \frac{U_t u - u}{t}, \quad u \in H$$

of $U_t, t \in \mathbb{R}$, which in a compact form reads $U_t = \mathrm{e}^{\mathrm{i}tA}$. An important example in quantum mechanics is $U_t = \mathrm{e}^{\mathrm{i}tH} U_0, t \in \mathbb{R}$ with H a self-adjoint Hamiltonian, which solves the Schrödinger equation $\mathrm{d}/\mathrm{d}t u = \mathrm{i}Hu$. The Lie–Trotter formula, which has important applications for Feynman path integrals, expresses the unitary semigroup generated by $A + B$, where A, B, and $A + B$ are self-adjoint on their respective domains as a strong limit

$$\mathrm{e}^{\mathrm{i}t(A+B)} = \lim_{t \to \infty} \left(\mathrm{e}^{\frac{\mathrm{i}tA}{n}} \mathrm{e}^{\frac{\mathrm{i}tB}{n}} \right)^n$$

On the other hand, positive operators on a Hilbert space $(H, \langle \cdot, \cdot \rangle_H)$ – that is, A self-adjoint and such that $\langle Au, u \rangle_H \geq 0 \quad \forall u \in D(A)$ – generate one-parameter semigroups $T_t = \mathrm{e}^{-tA}, t \geq 0$. Hille and Yosida proved that on a Hilbert space, strongly continuous contraction (i.e., $|||T_t||| \leq 1 \quad \forall t > 0$) semigroups such that $T_0 = \mathrm{Id}$ are in one-to-one correspondence with densely defined positive operators $A : D(A) \subset H \to H$ that are maximal (i.e., $I + A$ is onto), obtained as (minus the) infinitesimal generators

$$-Au = \lim_{t \to 0} \frac{T_t u - u}{t}, \quad u \in H$$

of the corresponding semigroups. Similarly, a positive densely defined self-adjoint operator A on a Hilbert space H gives rise to a densely defined closed symmetric sesquilinear form $(u, v) \mapsto \langle \sqrt{A} u, \sqrt{A} v \rangle_H$ (see next section for a definition of $\sqrt{A}$; $\langle \cdot, \cdot \rangle_H$ is the scalar product on H) and this map yields a one-to-one correspondence between operators and sesquilinear forms on H with the aforementioned properties, one of the starting points for the theory of Dirichlet forms. To a probability measure μ on a separable Banach space E, one can associate a densely defined closed symmetric sesquilinear form (it is in fact a Dirichlet form) on a Hilbert space H such that $E^* \subset H^* = H \subset E$, which in the particular case of the standard Wiener measure μ on the Wiener space $E = C([0, t])$ and with Hilbert space given by the Cameron–Martin space $H = H^1([0, t])$, is the bilinear form

$$(u, v) \mapsto \int \langle \bar{\nabla} u, \bar{\nabla} v \rangle_H$$

with $\bar{\nabla}$ the (closed) gradient of Malliavin calculus.

The operator $-\Delta$, where Δ is the Laplacian on $\mathbb{R}^n$, generates the heat-operator semigroup $\mathrm{e}^{-\Delta t}, t \geq 0$. It has a smooth kernel $K_t \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$ defined by

$$(\mathrm{e}^{-\Delta t} f)(x) = \int_{\mathbb{R}^n} K_t(x, y) f(y) \mathrm{d}y \quad \forall f \in C_0^\infty(\mathbb{R}^n)$$

and defines a smoothing operator, an operator that maps Sobolev function to smooth function. In general, a pseudodifferential operators A on an open subset U of $\mathbb{R}^n$ with symbol σ_A only has a distribution kernel

$$K_A(x, y) = \int_{\mathbb{R}^n} \mathrm{e}^{\mathrm{i}\langle x - y, \xi \rangle} \sigma(\xi) \mathrm{d}\xi$$

The kernel of the inverse Laplacian $(\Delta + m^2)^{-1}$ on $\mathbb{R}^n$ (the non-negative real number m^2 stands for the mass) called Green's function on $\mathbb{R}^n$, plays an essential role in the theory of Feynman graphs.

Spectral Theory

Spectral theory is the study of the distribution of the values of the complex parameter λ for which, given a linear operator A on a normed space E, the operator $A - \lambda I$ has an inverse and of the properties of this inverse when it exists, the resolvent $R(A, \lambda) = (A - \lambda I)^{-1}$ of A. The resolvent $\rho(A)$ of A is the set of complex numbers λ for which $A - \lambda I$ is invertible with densely defined bounded inverse. The spectrum $\mathrm{Sp}(A)$ of A is the complement in $\mathbb{C}$ of the resolvent; it consists of a union of three disjoint sets: the set of all complex numbers λ for which $A - \lambda I$ is not injective, called the point spectrum – such a λ is an eigenvalue of A with associated eigenfunction any $u \in D(A)$ such that $Au = \lambda u$; the set of points λ for which $A - \lambda I$ has a densely defined unbounded inverse $R(A, \lambda)$ called the continuous spectrum; and the set of points λ for which $A - \lambda I$ has a well-defined unbounded but not densely defined inverse $R(A, \lambda)$ called the residual spectrum.

A bounded operator has bounded spectrum and a self-adjoint operator A acting on a Hilbert space has *real spectrum and no residual spectrum since the* range of $A - \lambda I$ is dense. As a consequence of the

Fredholm alternative, the spectrum of a compact operator consists only of point spectrum; it is countable with accumulation point at 0. A Hamiltonian of a quantum mechanichal system can have both point and continuous spectra, but its point spectrum is of special interest because the corresponding eigenfunctions are stationary states of the system. As was first pointed out by Kac ("Can you hear the shape of a drum?"), the spectrum of an operator acting on functions can reflect the geometry of the space these functions are defined on, a starting point for many interesting and far-reaching questions in differential geometry.

A self-adjoint linear operator on a Hilbert space can be described in terms of a family of projections E_λ, $\lambda \in \mathbb{R}$ via the spectral representation

$$A = \int_{\mathrm{Sp}(A)} \lambda \mathrm{d}E_\lambda$$

Given a Borel real-valued function f on $\mathbb{R}$, the operator

$$f(A) = \int_{\mathrm{Sp}(A)} f(\lambda)\mathrm{d}E_\lambda$$

yields another self-adjoint operator. A positive operator A on a dense domain $D(A)$ of some Hilbert space $(H, \langle \cdot, \cdot \rangle_H)$ has non-negative spectrum and for any positive real number t, the map $\lambda \mapsto \mathrm{e}^{-t\lambda}$ gives the associated bounded heat-operator

$$\mathrm{e}^{-tA} = \int_{\mathrm{Sp}(A)} \mathrm{e}^{-t\lambda}\mathrm{d}E_\lambda$$

while the map $\lambda \mapsto \sqrt{\lambda}$ gives rise to a positive operator $\sqrt{A}$ such that $\sqrt{A}^2 = A$.

The resolvent can also be used to define new operators

$$f(A) = \frac{1}{2\mathrm{i}\pi} \int_C f(\lambda) R(A, \lambda)\mathrm{d}\lambda$$

from a linear operator via a Cauchy-type integral along a countour C around the spectrum; this way one defines complex powers A^{-z} of (essentially self-adjoint) positive elliptic pseudodiffferential operators which enter the definition of the zeta-function, $z \mapsto \zeta(A, z)$, of the operator A. The ζ-function is a useful tool to extend the ordinary determinant to ζ-determinants of self-adjoint elliptic operators, thereby providing an ansatz to give a meaning to partition functions in the path integral approach to quantum field theory.

Operator Algebras

Bounded linear operators on a Hilbert space H form an algebra $\mathcal{L}(H)$ closed for the operator norm with involution given by the adjoint operation $A \mapsto A^*$; it is a C^*-algebra, that is, an algebra over $\mathbb{C}$ with a norm $\| \cdot \|$ and an involution $*$ such that A is closed for this norm and such that $\|ab\| \leq \|a\|\|b\|$ and $\|a^*a\| = \|a\|^2$ for all $a, b \in A$ and by the Gelfand–Naimark theorem, every C^*-algebra is isomorphic to a sub-C^*-algebra of some $\mathcal{L}(H)$. The notion of spectrum extends from bounded operators to C^*-algebras; the spectrum $\mathrm{sp}(a)$ of an element a in a C^*-algebra A is a (compact) set of complex numbers such that $a - \lambda \cdot 1$ is not invertible. The notion of self-adjointness also extends $(a = a^*)$, and just as a self-adjoint operator $B \in \mathcal{L}(H)$ is non-negative (in which case its spectrum lies in $\mathbb{R}^+$) if and only if $B = A^*A$ for some bounded operator A, an element $b \in A$ is said to be non-negative if and only if $b = a^*a$ for some $a \in A$, in which case $\mathrm{sp}(a) \subset \mathbb{R}_0^+$.

The algebra $C(X)$ of continuous functions $f : X \to \mathbb{C}$ vanishing at infinity on some locally compact Hausdorff space X equipped with the supremum norm and the conjugation $f \mapsto \bar{f}$ is also a C^*-algebra and a prototype for abelian C^*-algebras, since Gelfand showed that every abelian C^*-algebra is isometrically isomorphic to $C(X)$, with X compact if the algebra is unital. To a C^*-algebra A, one can associate an abelian group $K_0(A)$ which is dual to the Grothendieck group $K^0(X)$ of isomorphism classes of vector bundles over a compact Hausdorff space X.

Compact operators on a Hilbert space H form the only proper two-sided ideal $\mathcal{K}(H)$ of the C^*-algebra $\mathcal{L}(H)$ which is closed for the operator norm topology on $\mathcal{L}(H)$. The quotient $\mathcal{L}(H)/\mathcal{K}(H)$ is called the Calkin space, after Calkin, who classified all two-sided ideals in $\mathcal{L}(H)$ for a separable Hilbert space H; one can set up a one-to-one correspondence between such ideals and certain sequence spaces. Corresponding to the Banach space $l^1(\mathbb{Z})$ of complex-valued sequences (u_n) such that $\sum_{n \in \mathbb{N}} |u_n| < \infty$, is the $*$-ideal $\mathcal{I}_1(H)$ of trace-class operators. The trace $\mathrm{tr}(A) = \sum_{n \in \mathbb{Z}} \langle A e_n, e_n \rangle_H$ of a negative operator $A \in \mathcal{L}(H)$ lies in $[0, +\infty]$ and is independent of the choice of the complete orthonormal basis $\{e_n, n \in \mathbb{Z}\}$ of H equipped with the inner product $\langle \cdot, \cdot \rangle_H$. $\mathcal{I}_1(H)$ is the Banach space of bounded linear operators on H such that $\|A\|_1 = \mathrm{tr}(|A|)$ is bounded. Given an (esssentially self-adjoint) positive differential operator D of order d acting on smooth functions on a closed n-dimensional Riemannian manifold M, its complex power D^{-z} is a trace class on the space of L^2-functions on M provided $\mathrm{Re}(z) > n/d$ and the corresponding trace $\mathrm{tr}(D^{-z})$ extends to a meromorphic function on the whole plane, the ζ-function $\zeta(D, z)$ which is holomorphic at 0.

More generally, Banach spaces $l^p(\mathbb{Z})$, $1 \leq p < \infty$, of complex-valued sequences $(u_n)_{n\in\mathbb{Z}}$ such that $\sum_{n\in\mathbb{Z}} |u_n|^p < \infty$ relate to Schatten ideals $\mathcal{I}_p(H)$, $1 \leq p < \infty$, where $\mathcal{I}_p(H)$ is the Banach space of bounded linear operators on H such that $\|A\|_p = (\mathrm{tr}(|A|^p))^{1/p}$ is bounded. Just as all l^p-sequences converge to 0, the Schatten ideals $\mathcal{I}_p(H)$ all lie in $\mathcal{K}(H)$ and we have $\cdots \subset \mathcal{I}_{p+1}(H) \subset \mathcal{I}_p(H) \subset \cdots \subset \mathcal{K}(H)$.

Compact operators and Schatten ideals are useful to extend index theory to a noncommutative context; a Fredholm module (H, F) over an involutive algebra A is given by an involutive representation π of A in a Hilbert space H and a self-adjoint bounded linear operator F on H such that $F^2 = \mathrm{Id}_H$ and the operator brackets $[F, \pi(a)]$ are compact for all $a \in A$. To a p-summable Fredholm module (H, F), that is, $[F, \pi(a)] \in \mathcal{I}_p(H)$ for all $a \in A$, one associates a representative τ of the Chern character $\mathrm{ch}^*(H, F)$ given by a cyclic cocycle on A, which pairs up with K-theory to build an integer-valued index map τ on K-theory.

Schatten ideals are also useful to investigate the geometry of infinite-dimensional spaces such as loop groups, for which the Hilbert–Schmidt operators (operators in $\mathcal{I}_2(H)$ are also called Hilbert–Schmidt operators) are particularly useful. A Hölder-type inequality shows that the product of two Hilbert–Schmidt operators is trace-class. Moreover, for any two Hilbert–Schmidt operators A and B, the "cyclicity property" that $\mathrm{tr}(AB) = \mathrm{tr}(BA)$ holds, and the sesquilinear form $(A, B) \mapsto \mathrm{tr}(AB^*)$ makes $\mathcal{L}_2(H)$ a Hilbert space.

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Introductory Article: Minkowski Spacetime and Special Relativity

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Introduction

Minkowski spacetime is generally regarded as the appropriate mathematical context within which to formulate those laws of physics that do not refer specifically to gravitational phenomena. Here we shall describe this context in rigorous terms, postulate what experience has shown to be its correct physical interpretation, and illustrate by means of examples its appropriateness for the formulation of physical laws.

Minkowski Spacetime and the Lorentz Group

Minkowski spacetime $\mathcal{M}$ is a four-dimensional real vector space on which is defined a bilinear form $g : \mathcal{M} \times \mathcal{M} \to \mathbb{R}$ that is symmetric ($g(v, w) = g(w, v)$ for all $v, w \in \mathcal{M}$) and nondegenerate ($g(v, w) = 0$ for all $w \in \mathcal{M}$ implies $v = 0$). Further, g has index 1, that is, there exists a basis $\{e_1, e_2, e_3, e_4\}$ for $\mathcal{M}$ with

$$g(e_a, e_b) = \eta_{ab} = \begin{cases} 1 & \text{if } a = b = 1, 2, 3 \\ -1 & \text{if } a = b = 4 \\ 0 & \text{if } a \neq b \end{cases}$$

g is called a Lorentz inner product for $\mathcal{M}$ and any basis of the type just described is an orthonormal basis for $\mathcal{M}$. We shall often write $v \cdot w$ for the value $g(v, w)$ of g on $(v, w) \in \mathcal{M} \times \mathcal{M}$. A vector $v \in \mathcal{M}$ is said to be spacelike, timelike, or null if $v \cdot v$ is positive, negative, or zero, respectively, and the set C_N of all null vectors is called the null cone in $\mathcal{M}$. If $\{e_1, e_2, e_3, e_4\}$ is an orthonormal basis and if we write $v = v^1 e_1 + v^2 e_2 + v^3 e_3 + v^4 e_4 = v^a e_a$ (using the Einstein summation convention, according to which a repeated index, one subscript and one superscript, is summed over its possible values) and $w = w^b e_b$, then

$$\begin{aligned} v \cdot w &= v^1 w^1 + v^2 w^2 + v^3 w^3 - v^4 w^4 \\ &= \eta_{ab} v^a w^b \end{aligned}$$

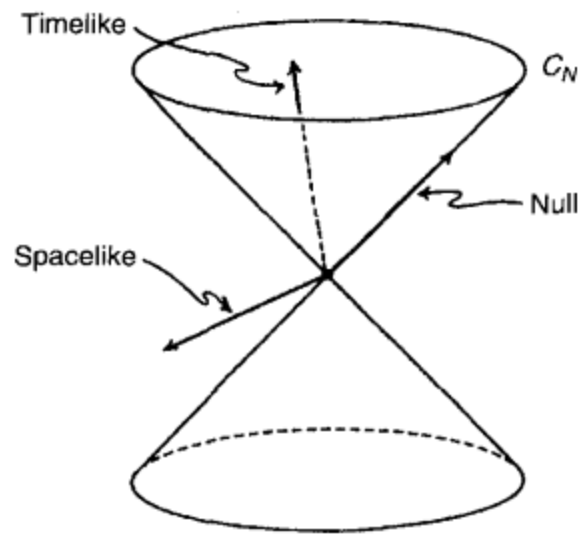

Figure 1 Spacelike, timelike and null vectors.

In particular, v is null if and only if

$$(v^4)^2 = (v^1)^2 + (v^2)^2 + (v^3)^2$$

(hence the name null "cone" for C_N). Timelike vectors are "inside" the null cone and spacelike vectors are "outside" (see **Figure 1**).

We select some orientation for the vector space $\mathcal{M}$ and will henceforth consider only oriented, orthonormal bases for $\mathcal{M}$. From the Schwartz inequality for $\mathbb{R}^3$, one can show (Naber 1992, theorem 1.3.1) that, if v is timelike and w is either timelike or null and nonzero, then $v \cdot w < 0$ if and only if $v^4 w^4 > 0$ in any orthonormal basis. In particular, one can define an equivalence relation on the set of all timelike vectors by decreeing that two such, v and w, are equivalent if and only if $v \cdot w < 0$. For reasons that will emerge shortly we then say that v and w have the same time orientation. There are precisely two equivalence classes, one of which we select and designate future directed. Timelike vectors in the other class are then called past directed. One can show (Naber 1992, section 1.3 and corollary 1.4.5) that this classification can be extended to nonzero null vectors as well (but not to spacelike vectors). We will call an oriented, orthonormal basis time oriented if its timelike vector e_4 is future directed and will consider only these in what follows. An oriented, time-oriented, orthonormal basis for $\mathcal{M}$ will be called an admissible basis. If $\{e_1, e_2, e_3, e_4\}$ and $\{\hat{e}_1, \hat{e}_2, \hat{e}_3, \hat{e}_4\}$ are two such bases and if we write

$$\begin{aligned} e_b &= \Lambda^1{}_b \hat{e}_1 + \Lambda^2{}_b \hat{e}_2 + \Lambda^3{}_b \hat{e}_3 + \Lambda^4{}_b \hat{e}_4 \\ &= \Lambda^a{}_b \hat{e}_a, \quad b = 1, 2, 3, 4 \end{aligned} \qquad [1]$$

then the matrix $\Lambda = (\Lambda^a{}_b)$ (a = row index, b = column index) can be shown to satisfy the following three conditions (Naber 1992, section 1.3):

1. (orthogonality) $\Lambda^{\mathrm{T}} \eta \Lambda = \eta$, where T means transpose and

$$\eta = (\eta_{ab}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

2. (orientability) $\det \Lambda = 1$, and
3. (time orientabiility) $\Lambda^4{}_4 \geq 1$.

We shall refer to any 4×4 matrix $\Lambda = (\Lambda^a{}_b)$ satisfying these three conditions as a Lorentz transformation (although one often sees the adjectives "proper" and "orthochronous" appended to emphasize conditions (2) and (3), respectively). The set $\mathcal{L}$ of all such matrices forms a group under matrix multiplication that we call simply the Lorentz group. It is a simple matter to show (Naber 1992, lemma 1.3.4) from the orthogonality condition (1) that, if $\Lambda^4{}_4 = 1$, then Λ must be of the form

$$\begin{pmatrix} & & & 0 \\ & (R^i{}_j) & & 0 \\ & & & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

where $(R^i{}_j)$ is an element of SO(3), that is, a 3×3 orthogonal matrix with determinant 1. The set $\mathcal{R}$ of all matrices of this form is a subgroup of $\mathcal{L}$ called the rotation subgroup. Although it will play no role in what we do here, it should be pointed out that in many applications (e.g., in particle physics) it is necessary to consider the larger group of transformations of $\mathcal{M}$ generated by the Lorentz group and spacetime translations ($x^a \to x^a + \Lambda^a$, for some constants $\Lambda^a, a = 1, 2, 3, 4$). This is called the inhomogeneous Lorentz group, or Poincaré group.

Physical Interpretation

For the purpose of describing how one is to think of Minkowski spacetime and the Lorentz group physically it will be convenient to distinguish (intuitively and terminologically, if not mathematically) between a "vector" in $\mathcal{M}$ and a "point" in $\mathcal{M}$ (the "tip" of a vector). The points in $\mathcal{M}$ are called events and are to be thought of as actual physical occurrences, albeit idealized as "point events" which have no spatial extension and no duration. One might picture, for example, an instantaneous collision, or explosion, or an "instant" in the history of some point material particle or photon ("particle of light").

Events are observed and identified by the assignment of coordinates. We will be interested in coordinates assigned in a very particular way by a

very particular type of observer. Specifically, our admissible observers preside over three-dimensional, right-handed, Cartesian spatial coordinate systems, relative to which photons always move along straight lines in any direction. With a single clock located at the origin, such an observer can determine the speed, c, of light *in vacuo* by the so-called Fizeau procedure (emit a photon from the origin when the clock there reads t_1, bounce it back from a mirror located at (x^1, x^2, x^3), receive the photon at the origin again when the clock there reads t_2 and set $c = 2\sqrt{(x^1)^2 + (x^2)^2 + (x^3)^2}/(t_2 - t_1)$). Now place an identical clock at each spatial point and synchronize them by emitting from the origin a spherical electromagnetic wave (photons in all directions) and setting the clock whose location is (x^1, x^2, x^3) to read $\sqrt{(x^1)^2 + (x^2)^2 + (x^3)^2}/c$ at the instant the wave arrives. An observer now assigns to an event the three spatial coordinates of the location at which it occurred in his coordinate system as well as the time reading on the clock at that location at the instant the event occurred. We shall assume also that our admissible observers are inertial in the sense of Newtonian mechanics (the trajectory of a particle on which no forces act, when described in terms of the coordinates just introduced, is a point or a straight line traversed at constant speed). It is an experimental fact (and quite a remarkable one) that all of these admissible observers (whether or not they are in relative motion) agree on the numerical value of the speed of light *in vacuo* ($c \approx 3.00 \times 10^{10}\,\mathrm{cm\,s^{-1}}$). We shall exploit this fact at the outset to have all of our admissible observers measure time in units of distance by simply multiplying their time coordinates t by c. The resulting time coordinate is denoted $x^4 = ct$. In these units all speeds are dimensionless and the speed of light *in vacuo* is 1.

In our mathematical model $\mathcal{M}$ of the world of events, this very subtle and complex notion of an admissible observer is fully identified with the conceptually very simple notion of an admissible basis $\{e_1, e_2, e_3, e_4\}$. If $x \in \mathcal{M}$ is an event and if we write $x = x^a e_a$, then (x^1, x^2, x^3) are the spatial and x^4 is the time coordinate supplied for x by the corresponding observer. If $\{\hat{e}_1, \hat{e}_2, \hat{e}_3, \hat{e}_4\}$ is another basis/observer related to $\{e_1, e_2, e_3, e_4\}$ by [1] and if we write $x = \hat{x}^a \hat{e}_a$, then

$$\hat{x}^a = \Lambda^a{}_b x^b, \quad a = 1, 2, 3, 4 \qquad [2]$$

Thus, Lorentz transformations relate the space and time coordinates supplied for any given event by two admissible observers. If $(\Lambda^a{}_b) \in \mathcal{R}$, then the two observers differ only in the orientation of their spatial coordinate axes. On the other hand, for any real number θ one can define an element $L(\theta)$ of $\mathcal{L}$ by

$$L(\theta) = \begin{pmatrix} \cosh\theta & 0 & 0 & -\sinh\theta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sinh\theta & 0 & 0 & \cosh\theta \end{pmatrix} \qquad [3]$$

and, if two admissible bases are related by this Lorentz transformation, then the coordinate transformation [2] becomes

$$\begin{aligned} \hat{x}^1 &= (\cosh\theta)\, x^1 - (\sinh\theta)\, x^4 \\ \hat{x}^2 &= x^2 \\ \hat{x}^3 &= x^3 \\ \hat{x}^4 &= -(\sinh\theta)\, x^1 + (\cosh\theta)\, x^4 \end{aligned} \qquad [4]$$

Letting $\beta = \tanh\theta$ (so that $-1 < \beta < 1$) and suppressing $\hat{x}^2 = x^2$ and $\hat{x}^3 = x^3$, one obtains

$$\begin{aligned} \hat{x}^1 &= \frac{1}{\sqrt{1-\beta^2}} x^1 - \frac{\beta}{\sqrt{1-\beta^2}} x^4 \\ \hat{x}^4 &= -\frac{\beta}{\sqrt{1-\beta^2}} x^1 + \frac{1}{\sqrt{1-\beta^2}} x^4 \end{aligned} \qquad [5]$$

This corresponds to two observers whose spatial axes are oriented as shown in **Figure 2** with the hatted coordinate system moving along the common x^1-, $\hat{x}^1$-axis with speed $|\beta|$, to the right if $\beta > 0$ and to the left if $\beta < 0$.

We remark that, reverting to traditional time units, $\beta = v/c$, where $|v|$ is the relative speed of the two coordinate systems, and [5] becomes what is generally referred to as a "Lorentz transformation" in elementary expositions of special relativity, that is,

$$\begin{aligned} \hat{x}^1 &= \frac{x^1 - vt}{\sqrt{1 - v^2/c^2}} \\ \hat{t} &= \frac{t - (v/c^2)x^1}{\sqrt{1 - v^2/c^2}} \end{aligned} \qquad [6]$$

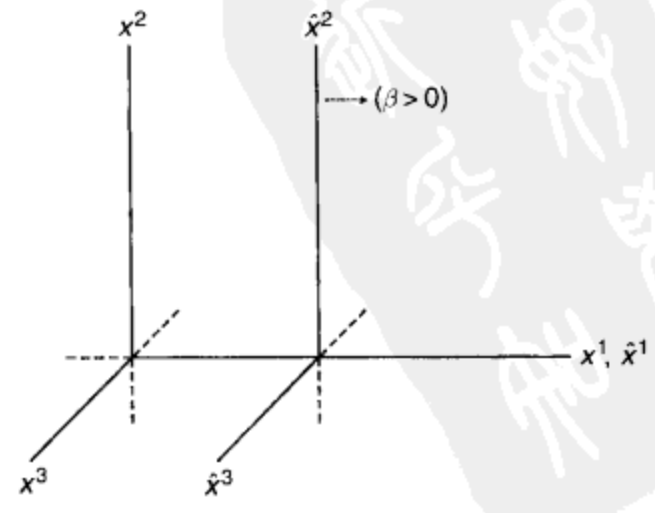

Figure 2 Observers in standard configuration.

There is a sense in which, to understand the kinematic effects of special relativity, it is enough to restrict one's attention to the so-called special Lorentz transformations $L(\theta)$. Specifically, one can show (Naber 1992, theorem 1.3.5) that if $\Lambda \in \mathcal{L}$ is any Lorentz transformation, then there exists a real number θ and two rotations $R_1, R_2 \in \mathcal{R}$ such that $\Lambda = R_1 L(\theta) R_2$. Since R_1 and R_2 involve no relative motion, all of the kinematics is contained in $L(\theta)$. We shall explore these kinematic effects in more detail shortly.

Now suppose that x and x_0 are two distinct events in $\mathcal{M}$ and consider the displacement vector $x - x_0$ from x_0 to x. If $\{e_1, e_2, e_3, e_4\}$ is an admissible basis and if we write $x = x^a e_a$ and $x_0 = x_0^a e_a$, then $x - x_0 = (x^a - x_0^a)e_a = \Delta x^a e_a$. If $x - x_0$ is null, then

$$(\Delta x^1)^2 + (\Delta x^2)^2 + (\Delta x^3)^2 = (\Delta x^4)^2$$

so the spatial separation of the two events is equal to the distance light would travel during the time lapse between the events. The same must be true in any other admissible basis since Lorentz transformations are the matrices of linear maps that preserve the Lorentz inner product. Consequently, all admissible observers agree that x_0 and x are "connectible by a photon." They even agree as to which of the two events is to be regarded as the "emission" of the photon and which is to be regarded as its "reception" since one can show (Naber 1992, theorem 1.3.3) that, when a vector is either timelike or null and nonzero, the sign of its fourth coordinate is the same in every admissible basis (because $\Lambda^4{}_4 \geq 1$). Thus, $x^4 - x_0^4$ is either positive for all admissible observers (x_0 occurred before x) or negative for all admissible observers (x_0 occurred after x). Since photons move along straight lines in admissible coordinate systems we adopt the following terminology. If $x_0, x \in \mathcal{M}$ are such that $x - x_0$ is null, then the straight line in $\mathcal{M}$ containing x_0 and x is called the world line of a photon in $\mathcal{M}$ and is to be thought of as the set of all events in the history of some particle of light that "experiences" both x_0 and x.

Let us now suppose instead that $x - x_0$ is timelike. Then, in any admissible basis,

$$(\Delta x^1)^2 + (\Delta x^2)^2 + (\Delta x^3)^2 < (\Delta x^4)^2$$

so the spatial separation of x_0 and x is less than the distance light would travel during the time lapse between the events. In this case, one can prove (Naber 1992, section 1.4) that there exists an admissible basis $\{\hat{e}_1, \hat{e}_2, \hat{e}_3, \hat{e}_4\}$ in which $\Delta\hat{x}^1 = \Delta\hat{x}^2 = \Delta\hat{x}^3 = 0$, that is, there is an admissible observer for whom the two events occur at the same spatial location, one after the other. Thinking of this location as occupied by some material object (e.g., the observer's clock situated at that point) we find that the events x_0 and x are both "experienced" by this material particle and that, moreover, $\sqrt{|g(x - x_0, x - x_0)|}$ is just the time lapse between the events recorded by a clock carried along by this material particle. To any other admissible observer this material particle appears "free" (not subject to forces) because it moves on a straight line with constant speed. This leads us to the following definitions. If $x_0, x \in \mathcal{M}$ are such that $x - x_0$ is timelike, then the straight line in $\mathcal{M}$ containing x_0 and x is called the world line of a free material particle in $\mathcal{M}$ and $\sqrt{|g(x - x_0, x - x_0)|}$, usually written $\tau(x - x_0)$, or simply $\Delta\tau$, is the proper time separation of x_0 and x. One can think of $\tau(x - x_0)$ as a sort of "length" for $x - x_0$ measured, however, by a clock carried along by a free material particle that experiences both x_0 and x. It is an odd sort of length, however, since it satisfies not the usual triangle inequality, but the following "reversed" version.

Reversed triangle inequality (Naber 1992, theorem 1.4.2) *Let x_0, x and y be events in $\mathcal{M}$ for which $y - x$ and $x - x_0$ are timelike with the same time orientation. Then $y - x_0 = (y - x) + (x - x_0)$ is timelike and*

$$\tau(y - x_0) \geq \tau(y - x) + \tau(x - x_0) \qquad [7]$$

with equality holding if and only if $y - x$ and $x - x_0$ are linearly dependent.

The sense of the inequality in [7] has interesting consequences about which we will have more to say shortly.

Finally, let us suppose that $x - x_0$ is spacelike. Then, in any admissible basis

$$(\Delta x^1)^2 + (\Delta x^2)^2 + (\Delta x^3)^2 > (\Delta x^4)^2$$

so the spatial separation of x_0 and x is greater than the distance light could travel during the time lapse that separates them. There is clearly no admissible observer for whom the events occur at the same location. No free material particle (or even photon) can experience both x_0 and x. However, one can show (Naber 1992, section 1.5) that, given any real number T (positive, negative, or zero), one can find an admissible basis $\{\hat{e}_1, \hat{e}_2, \hat{e}_3, \hat{e}_4\}$ in which $\Delta\hat{x}^4 = T$. Some admissible observers will judge the events simultaneous, some will assert that x_0 occurred before x, and others will reverse the order. Temporal order, cause and effect, have no meaning for such pairs of events. For those admissible observers for whom the events are simultaneous ($\Delta\hat{x}^4 = 0$), the quantity $\sqrt{g(x - x_0, x - x_0)}$ is the distance between them and for this reason this quantity is called the proper spatial separation of x_0 and x (whenever $x - x_0$ is spacelike).

For any two events $x_0, x \in \mathcal{M}$, $g(x - x_0, x - x_0)$ is given in any admissible basis by $(\Delta x^1)^2 + (\Delta x^2)^2 + (\Delta x^3)^2 - (\Delta x^4)^2$ and is called the interval separating x_0 and x. It is the closest analog in Minkowskian geometry to the (squared) length in Euclidean geometry. It can, however, assume any real value depending on the physical relationship between the events x_0 and x. Historically, of course, it was the various physical interpretations of this interval that we have just described which led Minkowski (Einstein *et al.* 1958) to the introduction of the structure that bears his name.

Kinematic Effects

All of the well-known kinematic effects of special relativity (the addition of velocities formula, the relativity of simultaneity, time dilation, and length contraction) follow easily from what we have done. Because it eases visualization and because, as we mentioned earlier, it suffices to do so, we will limit our discussion to the special Lorentz transformations.

Let θ_1 and θ_2 be two real numbers and consider the corresponding elements $L(\theta_1)$ and $L(\theta_2)$ of $\mathcal{L}$ defined by [3]. Sum formulas for $\sinh\theta$ and $\cosh\theta$ imply that $L(\theta_1)L(\theta_2) = L(\theta_1 + \theta_2)$. Defining $\beta_i = \tanh\theta_i, i = 1, 2$, and $\beta = \tanh(\theta_1 + \theta_2)$, the sum formula for $\tanh\theta$ then gives

$$\beta = \frac{\beta_1 + \beta_2}{1 + \beta_1\beta_2} \qquad [8]$$

The physical interpretation is simple. One has three admissible observers whose spatial axes are related in the manner shown in **Figure 2**. If the speed of the second relative to the first is β_1 and the speed of the third relative to the second is β_2, then the speed of the third relative to the first is not $\beta_1 + \beta_2$ as a Newtonian predisposition would lead one to expect, but rather β, given by [8]. This is the relativistic addition of velocities formula.

We have seen already that, when the interval between x_0 and x is spacelike, the events will be judged simultaneous by some admissible observers, but not by others. Indeed, if $\Delta x^4 = 0$ and the observers are related by [5], then $\Delta\hat{x}^4 = -(\beta/\sqrt{1-\beta^2})\Delta x^1 = -\beta\Delta\hat{x}^1$, which will not be zero unless $\beta = 0$ and so there is no relative motion ($\Delta\hat{x}^1$ cannot be zero since then $\Delta\hat{x}^a = 0$ for $a = 1, 2, 3, 4$ and $x = x_0$). This phenomenon is called the relativity of simultaneity and we now construct a simple geometrical representation of it.

Select two perpendicular lines in the plane to represent the x^1- and x^4-axes (the Euclidean orthogonality of the lines has no physical significance and is unnecessary, but makes the pictures easier to draw). The $\hat{x}^1$-axis will be represented by the straight line $\hat{x}^4 = 0$ which, from [5], is given by $x^4 = \beta x^1$ (in **Figure 3** we have assumed that $\beta > 0$). Similarly, the $\hat{x}^4$-axis is identified with the line $x^4 = (1/\beta)x^1$. Since Lorentz transformations leave the Lorentz inner product invariant, the hyperbolas $(x^1)^2 - (x^4)^2 = k$ coincide with $(\hat{x}^1)^2 - (\hat{x}^4)^2 = k$ and we calibrate the axes accordingly, for example, the branch of $(x^1)^2 - (x^4)^2 = 1$ with $x^1 > 0$ intersects the x^1-axis at the point $(x^1, x^4) = (1, 0)$ and intersects the $\hat{x}^1$-axis at the point $(\hat{x}^1, \hat{x}^4) = (1, 0)$. This necessitates a different scale on the hatted and unhatted axes, but one can show (Naber 1992, section 1.3) that, with this calibration, all coordinates can be obtained geometrically by projecting parallel to the opposite axis (e.g., the x^4- and $\hat{x}^4$-coordinates of an event result from projecting parallel to the x^1- and $\hat{x}^1$-axes, respectively).

Thus, a line of simultaneity in the hatted (respectively, unhatted) coordinates is parallel to the $\hat{x}^1$- (respectively, x^1-) axis so that, in general, a pair of events lying on one will not lie on the other (note, however, that these lines are "really" three-dimensional hyperplanes so what appears to be a point of intersection is actually a two-dimensional "plane of agreement", any two events in which are judged simultaneous by both observers).

For any two events whatsoever the relationship between the time lapse $\Delta\hat{x}^4$ in the hatted coordinates and the time lapse Δx^4 in the unhatted coordinates is, from [5],

$$\Delta\hat{x}^4 = -\frac{\beta}{\sqrt{1-\beta^2}}\Delta x^1 + \frac{1}{\sqrt{1-\beta^2}}\Delta x^4$$

so the two are generally not equal. Consider, in particular, two events on the world line of a point at rest in the unhatted coordinate system, for

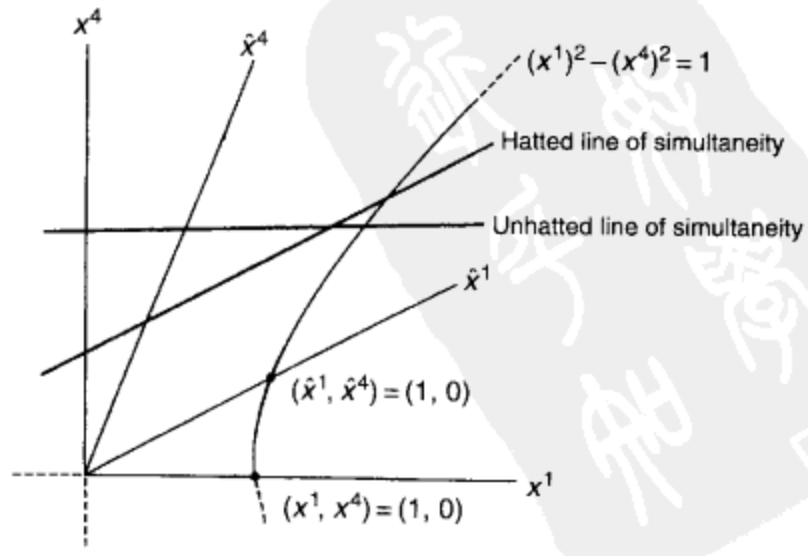

Figure 3 Relativity of simultaneity.

example, two readings on the clock at rest at the origin in this system. Then $\Delta x^1 = 0$ so

$$\Delta \hat{x}^4 = \frac{1}{\sqrt{1-\beta^2}} \Delta x^4 > \Delta x^4$$

This effect is entirely symmetrical since, if $\Delta \hat{x}^1 = 0$, then [5] implies

$$\Delta x^4 = \frac{1}{\sqrt{1-\beta^2}} \Delta \hat{x}^4 > \Delta \hat{x}^4$$

Each observer judges the other's clocks to be running slow. This phenomenon is called time dilation and is clearly visible in the spacetime diagram in **Figure 4** (e.g., both observers agree on the time reading "0" for the clock at the origin of the unhatted system, but the line $\hat{x}^4 = 1$ intersects the world line of the clock, i.e., the x^4-axis, at a point below $(x^1, x^4) = (0, 1)$).

We should emphasize that this phenomenon is quite "real" in the physical sense. For example, certain types of elementary particles (mesons) found in cosmic radiation are so short-lived (at rest) that, even if they could travel at the speed of light, the time required to traverse our atmosphere would be some ten times their normal life span. They should not be able to reach the earth, but they do. Time dilation "keeps them young" in the sense that what seems a normal life time to the meson appears much longer to us.

Finally, since admissible observers generally disagree on which events are simultaneous and since the only way to measure the "length" of a moving object (say, a measuring rod) is to locate its end points "simultaneously," it should come as no surprise that length, like simultaneity, and time, depends on the admissible observer measuring it. Specifically, let us consider a measuring rod lying at rest along the $\hat{x}^1$-axis of the hatted coordinate

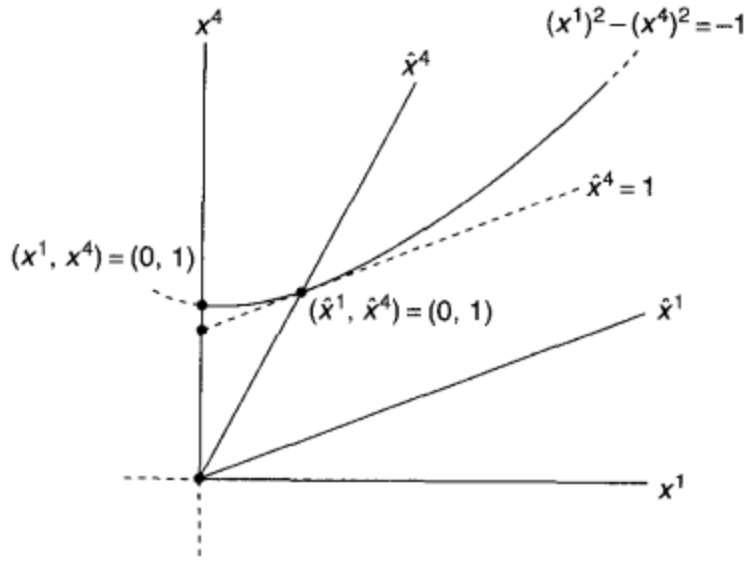

Figure 4 Time dilation.

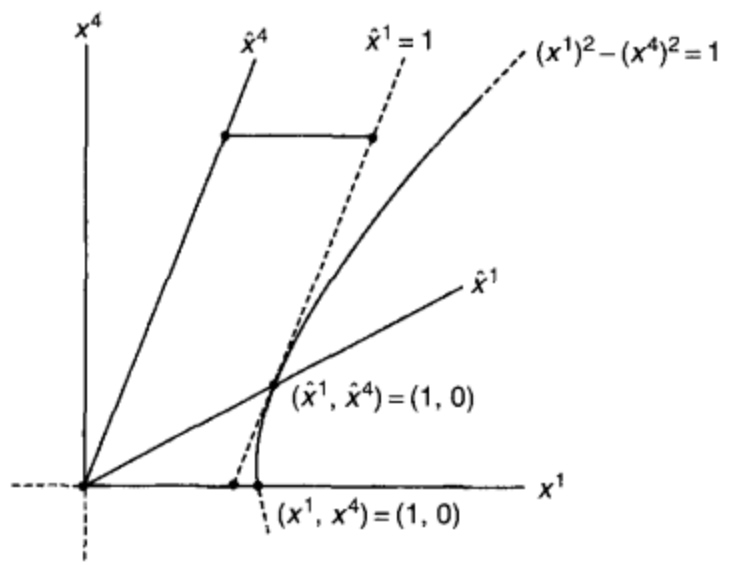

Figure 5 Length contraction.

system. Its "length" in this coordinate system is $\Delta \hat{x}^1$. The world lines of its end points are two straight lines parallel to the $\hat{x}^4$-axis. If the unhatted observer locates two events on these world lines "simultaneously" their coordinates will satisfy $\Delta x^4 = 0$ and, by [5] $\Delta \hat{x}^1 = (1/\sqrt{1-\beta^2})\Delta x^1$ so

$$\Delta x^1 = \sqrt{1-\beta^2}\, \Delta \hat{x}^1 < \Delta \hat{x}^1$$

and the moving measuring rod appears contracted in its direction of motion by a factor of $\sqrt{1-\beta^2}$. As for time dilation, this phenomenon, known as length contraction, is entirely symmetrical, quite real, and clearly visible in a spacetime diagram (**Figure 5**).

The Relativity Principle

We have found that admissible observers can disagree about some rather startling things (whether or not two events are simultaneous, the time lapse between two events even when no one thinks they are simultaneous, and the length of a measuring rod). This would be a matter of no concern at all, of course, if one could determine, in any given situation, who was really right. Surely, two events are either simultaneous or they are not and we need only sort out which admissible observer has the correct view of the situation? Unfortunately (or fortunately, depending on one's point of view) this distinction between the judgments made by different admissible observers is precisely what physics forbids.

The relativity principle (Einstein *et al.* 1958). *All admissible observers are completely equivalent for the formulation of the laws of physics.*

We must be clear that this is not a mathematical statement. It is rather a statement about the physical world around us and how it should be described, gleaned from observations, some of which are

complex and subtle and some of which are commonplace (a passenger in a smooth, quiet airplane traveling at constant groundspeed cannot "feel" his motion relative to the earth). It is a powerful guide for constructing the laws of relativistic physics, but even more fundamentally it prohibits us from regarding any particular admissible observer as having a privileged view of the universe. In particular, we are forbidden from attaching any objective significance to such questions as, "were the two supernovae simultaneous?", "How long did the meson survive?", and "What is the distance between the Crab Nebula and Alpha Centauri?" This is severe, but one must deal with it.

Particles and 4-Momentum

If $I \subseteq \mathbb{R}$ is an interval, then a map $\alpha : I \to \mathcal{M}$ is a curve in $\mathcal{M}$. Relative to any admissible basis we can write

$$\alpha(\xi) = x^a(\xi)\, e_a$$

for each $\xi \in I$. We shall assume that α is smooth in the sense that each $x^a(\xi), a = 1, 2, 3, 4$, is infinitely differentiable (C^∞) on I and the velocity vector

$$\alpha'(\xi) = \frac{dx^a}{d\xi} e_a$$

is nonzero for every $\xi \in I$ (we adopt the usual custom, in a vector space, of identifying the tangent space at each point with the vector space itself). This definition of smoothness clearly does not depend on the choice of admissible basis for $\mathcal{M}$. The curve α is said to be spacelike, timelike, or null if

$$\alpha'(\xi) \cdot \alpha'(\xi) = \eta_{ab} \frac{dx^a}{d\xi} \frac{dx^b}{d\xi}$$

is positive, negative, or zero, respectively, for each $\xi \in I$. A timelike curve α for which $\alpha'(\xi)$ is future directed for each $\xi \in I$ is called a timelike world line and its image is identified with the set of all events in the history of some (not necessarily free) point material particle. If $I = [\xi_0, \xi_1]$ and $\alpha : [\xi_0, \xi_1] \to \mathcal{M}$ is a timelike world line, then the proper time length of α is defined by

$$L(\alpha) = \int_{\xi_0}^{\xi_1} \sqrt{|g(\alpha'(\xi), \alpha'(\xi))|}\, d\xi$$
$$= \int_{\xi_0}^{\xi_1} \sqrt{-\eta_{ab} \frac{dx^a}{d\xi} \frac{dx^b}{d\xi}}\, d\xi$$

and interpreted as the time lapse between the events $\alpha(\xi_0)$ and $\alpha(\xi_1)$ as recorded by a clock carried along by the particle whose world line is α. This interpretation is easily motivated by writing out a Riemann sum approximation to the integral and appealing to our interpretation of the proper time separation $\Delta\tau = \sqrt{-\eta_{ab}\, \Delta x^a\, \Delta x^b}$. There are subtleties, however, both mathematical and physical (Naber 1992, section 1.4). The mathematical ones are addressed by the following result (which combines theorems 1.4.6 and 1.4.8 of Naber (1992)).

Theorem *Let x_0 and x be two events in $\mathcal{M}$. Then $x - x_0$ is timelike and future directed if and only if there exists a timelike world line $\alpha : [\xi_0, \xi_1] \to \mathcal{M}$ in $\mathcal{M}$ with $\alpha(\xi_0) = x_0$ and $\alpha(\xi_1) = x$ and, in this case,*

$$L(\alpha) \leq \tau(x - x_0) \qquad [9]$$

with equality holding if and only if α is a parametrization of a timelike straight line.

The inequality [9] asserts that if two material particles experience both x_0 and x, then the one that is free (and so can be regarded as at rest in some admissible coordinate system) has longer to wait for the occurrence of the second event (moving clocks run slow). For many years this basically obvious fact was christened "The Twin Paradox."

Just as a smooth curve in Euclidean space has an arc length parametrization, so a timelike world line has a proper time parametrization defined as follows. For each ξ in $[\xi_0, \xi_1]$ let

$$\tau = \tau(\xi) = \int_{\xi_0}^{\xi} \sqrt{|g(\alpha'(\zeta), \alpha'(\zeta))|}\, d\zeta$$

(the proper time length of α from $\alpha(\xi_0)$ to $\alpha(\xi)$). Then $\tau = \tau(\xi)$ has a smooth inverse $\xi = \xi(\tau)$ so α can be reparametrized by τ. We will abuse our notation slightly and write

$$\alpha(\tau) = x^a(\tau) e_a$$

The velocity vector with this parametrization is denoted

$$U = U(\tau) = \frac{dx^a}{d\tau} e_a$$

called the 4-velocity of the world line and is the unit tangent vector field to α, that is,

$$U(\tau) \cdot U(\tau) = -1 \qquad [10]$$

for each τ. An admissible observer is, of course, more likely to parametrize a world line by his own time coordinate x^4. Then

$$\alpha'(x^4) = \frac{dx^1}{dx^4} e_1 + \frac{dx^2}{dx^4} e_2 + \frac{dx^3}{dx^4} e_3 + e_4$$

so

$$|g(\alpha'(x^4), \alpha'(x^4))| = 1 - \|V\|^2$$

where

$$\|V\| = \sqrt{\left(\frac{dx^1}{dx^4}\right)^2 + \left(\frac{dx^2}{dx^4}\right)^2 + \left(\frac{dx^3}{dx^4}\right)^2}$$

is the usual magnitude of the particle's velocity vector

$$\begin{aligned} V &= V(x^4) \\ &= \frac{dx^1}{dx^4}e_1 + \frac{dx^2}{dx^4}e_2 + \frac{dx^3}{dx^4}e_3 \\ &= V^i e_i \end{aligned}$$

in the given admissible coordinate system. One finds then that

$$U = \left(1 - \|V\|^2\right)^{-1/2}(V + e_4) \qquad [11]$$

We shall identify a material particle in $\mathcal{M}$ with a pair (α, m), where α is a timelike world line and m is a positive constant called the particle's proper mass (or rest mass). If each $dx^a/d\xi$, $a = 1, 2, 3, 4$, is constant, then (α, m) is a free material particle with proper mass m. The 4-momentum of (α, m) is defined by $P = mU$. Thus,

$$P \cdot P = -m^2 \qquad [12]$$

In any admissible basis we write

$$\begin{aligned} P &= P^a e_a = mU^a e_a = m\frac{dx^a}{d\tau}e_a \\ &= m\left(1 - \|V\|^2\right)^{-1/2}(V + e_4) \end{aligned} \qquad [13]$$

The "spatial part" of P in these coordinates is

$$\boldsymbol{P} = \frac{m}{\sqrt{1 - \|V\|^2}}V$$

which, for $\|V\| \ll 1$, is approximately $m\boldsymbol{V}$. Identifying m with the inertial mass of Newtonian mechanics (measured by an observer for whom the particle's speed is small), this is simply the classical momentum of the particle. Somewhat more explicitly, if one expands $1/\sqrt{1 - \|V\|^2}$ by the Binomial Theorem one finds that

$$\begin{aligned} P^i &= \frac{m}{\sqrt{1 - \|V\|^2}}V^i \\ &= mV^i + \frac{1}{2}mV^i\|V\|^2 + \cdots, \quad i = 1, 2, 3 \end{aligned} \qquad [14]$$

which gives the components of the classical momentum plus "relativistic corrections." In order to preserve a formal similarity with Newtonian mechanics one often sees $m/\sqrt{1 - \|V\|^2}$ referred to as the "relativistic mass" of the particle, but we shall avoid this terminology. The fourth component of P is given by

$$\begin{aligned} P^4 &= -P \cdot e_4 \\ &= \frac{m}{\sqrt{1 - \|V\|^2}} = m + \frac{1}{2}m\|V\|^2 + \cdots \end{aligned} \qquad [15]$$

The appearance of the term $(1/2)m\|V\|^2$ corresponding to the Newtonian kinetic energy suggests that P^4 be denoted E and called the total relativistic energy measured by the given admissible observer for the particle:

$$E = -P \cdot e_4 \qquad [16]$$

Now, one must understand that the concept of "energy" in physics is a subtle one and simply giving $-P \cdot e_4$ this name does not ensure that there is any physical content. Whether or not the name is appropriate can only be determined experimentally. In particular, one should ask if the appearance of the term m in [15] is consistent with the view that P^4 represents the "energy" of the particle. Observe that if $\|V\| = 0$ (i.e., if the particle is at rest relative to the given observer), then [15] gives

$$E = m \; (= mc^2, \text{ in standard units}) \qquad [17]$$

which we interpret as saying that, even when the particle is at rest, it still has energy. If this is really "energy" in the physical sense, then it should be possible to liberate and use it. That this is, indeed, possible has, of course, been rather convincingly demonstrated.

Next we observe that not only material particles, but also photons possess "momentum" and "energy" and therefore should have 4-momentum (witness, e.g., the photoelectric effect in which photons collide with and eject electrons from their orbits in an atom). Unlike a material particle, however, a photon's characteristic feature is not proper mass, but frequency ν, or wavelength $\lambda = 1/\nu$, related to its energy $\mathcal{E}$ by $\mathcal{E} = h\nu$ (h being Planck's constant) and these are highly observer dependent (Doppler effect). There is, moreover, no "proper frequency" analogous to "proper mass" since there is no admissible observer for whom the photon is at rest. In an attempt to model these features we consider a point $x_0 \in \mathcal{M}$, a future directed null vector N and an interval $I \subseteq \mathbb{R}$. The curve $\alpha : I \to \mathcal{M}$ defined by

$$\alpha(\xi) = x_0 + \xi N \qquad [18]$$

is a parametrization of the world line of a photon through x_0. Being null, N can be written in any admissible basis as

$$N = (-N \cdot e_4)(\boldsymbol{d} + e_4) \qquad [19]$$

where

$$\boldsymbol{d} = \Big[(N \cdot e_1)^2 + (N \cdot e_2)^2 + (N \cdot e_3)^2\Big]^{-1/2}\Big[(N \cdot e_1)e_1 + (N \cdot e_2)e_2 + (N \cdot e_3)e_3\Big] \qquad [20]$$

is the direction vector of the world line in the corresponding spatial coordinate system. Now, by analogy with [16], we define a photon in $\mathcal{M}$ to be a curve in $\mathcal{M}$ of the form [18], take N to be its 4-momentum and define the energy $\mathcal{E}$ of the photon in the admissible basis $\{e_1, e_2, e_3, e_4\}$ by

$$\mathcal{E} = -N \cdot e_4 \qquad [21]$$

Then, by [19],

$$N = \mathcal{E}(\boldsymbol{d} + e_4) \qquad [22]$$

The corresponding frequency ν and wavelength λ are then defined by $\nu = \mathcal{E}/h$ and $\lambda = 1/\nu$. In another admissible basis, one has $N = \hat{\mathcal{E}}(\hat{\boldsymbol{d}} + \hat{e}_4)$, where $\hat{\boldsymbol{d}}$ and $\hat{\mathcal{E}}$ are defined by the hatted versions of [20] and [21]. One can then show (Naber 1992, section 1.8) that

$$\frac{\hat{\mathcal{E}}}{\mathcal{E}} = \frac{\hat{\nu}}{\nu} = \frac{1 - \beta\cos\theta}{\sqrt{1-\beta^2}} = (1 - \beta\cos\theta) + \frac{1}{2}\beta^2(1 - \beta\cos\theta) + \cdots \qquad [23]$$

where β is the relative speed of the two spatial coordinate systems and θ is the angle (in the unhatted spatial coordinate system) between the direction $\boldsymbol{d}$ of the photon and the direction of motion of the hatted spatial coordinate system. Equation [23] is the formula for the relativistic Doppler effect with the first term in the series being the classical formula.

We conclude this section by examining a few simple interactions between particles of the sort modeled by our definitions, assuming only that 4-momentum is conserved in the interaction. For convenience, we will use the term free particle to refer to either a free material particle or a photon. If $\mathcal{A}$ is a finite set of free particles, then each element of $\mathcal{A}$ has a unique 4-momentum which is a future-directed timelike or null vector. The sum of any such collection of vectors is timelike and future directed, except when all of the vectors are null and parallel, in which case the sum is null and future directed (Naber 1992, lemma 1.4.3). We call this sum the total 4-momentum of $\mathcal{A}$. Now we formulate a definition which is intended to model a finite set of free particles colliding at some event with a (perhaps new) set of free particles emerging from the collision (e.g., an electron and proton collide, with a neutron and neutrino emerging from the collision). A contact interaction in $\mathcal{M}$ is a triple $(\mathcal{A}, x, \tilde{\mathcal{A}})$, where $\mathcal{A}$ and $\tilde{\mathcal{A}}$ are two finite sets of free particles, neither of which contains a pair of particles with linearly dependent 4-momenta (which would presumably be physically indistinguishable) and $x \in \mathcal{M}$ is an event such that

1. x is the terminal point of all of the particles in $\mathcal{A}$ (i.e., for each world line $\alpha : [\xi_0, \xi_1] \to \mathcal{M}$ of a particle in $\mathcal{A}$, $\alpha(\xi_1) = x$);
2. x is the initial point of all the particles in $\tilde{\mathcal{A}}$, and
3. the total 4-momentum of $\mathcal{A}$ equals the total 4-momentum of $\tilde{\mathcal{A}}$.

Properly (3) is called the conservation of 4-momentum. If $\mathcal{A}$ consists of a single free particle, then $(\mathcal{A}, x, \tilde{\mathcal{A}})$ is called a decay (e.g., a neutron decays into a proton, an electron and an antineutrino).

Consider, for example, an interaction $(\mathcal{A}, x, \tilde{\mathcal{A}})$ for which $\tilde{\mathcal{A}}$ consists of a single photon. The total 4-momentum of $\tilde{\mathcal{A}}$ is null so the same must be true of $\mathcal{A}$. Since the 4-momenta of the individual particles in $\mathcal{A}$ are timelike or null and future directed their sum can be null only if they are, in fact, all null and parallel. Since $\mathcal{A}$ cannot contain distinct photons with parallel 4-momenta, it must consist of a single photon which, by (3), must have the same 4-momentum as the photon in $\tilde{\mathcal{A}}$. In essence, "nothing happened at x." We conclude that *no nontrivial interaction of the type modeled by our definition can result in a single photon and nothing else*. Reversing the roles of $\mathcal{A}$ and $\tilde{\mathcal{A}}$ shows that, if 4-momentum is to be conserved, *a photon cannot decay*.

Next let us consider the decay of a single material particle into two material particles, for example, the spontaneous disintegration of an atom through α-emission. Thus, we consider a contact interaction $(\mathcal{A}, x, \tilde{\mathcal{A}})$ in which $\mathcal{A}$ consists of a single free material particle of proper mass m_0 and $\tilde{\mathcal{A}}$ consists of two free material particles with proper masses m_1 and m_2. Let P_0, P_1, and P_2 be the 4-momenta of the particles of proper mass m_0, m_1, and m_2, respectively. Then $P_0 = P_1 + P_2$. Appealing to the "reversed triangle inequality," the fact that P_1 and P_2 are linearly independent and future directed, and [12] we conclude that

$$m_0 > m_1 + m_2 \qquad [23]$$

The excess mass $m_0 - (m_1 + m_2)$ of the initial particle is regarded, via [17], as a measure of the amount of energy required to split m_0 into two pieces. Stated somewhat differently, when the two particles in $\tilde{\mathcal{A}}$ were held together to form the single particle in $\mathcal{A}$, the "binding energy" contributed to the mass of this latter particle.

Reversing the roles of $\mathcal{A}$ and $\tilde{\mathcal{A}}$ in the last example gives a contact interaction modelling an inelastic collision (two free material particles with masses m_1 and m_2 collide and coalesce to form a third of mass m_0). The inequality [23] remains true, of course, and a somewhat more detailed analysis (Naber 1992, section 1.8) yields an approximate formula for $m_0 - (m_1 + m_2)$ which can be compared (favorably) with the Newtonian formula for the loss in kinetic energy that results from the collision (energy which, classically, is viewed as taking the form of heat in the combined particle). An analysis of the interaction in which both $\mathcal{A}$ and $\tilde{\mathcal{A}}$ consist of an electron and a photon yields (Naber 1992, section 1.8) a formula for the so-called Compton effect. Many more such examples of this sort are treated in great detail in Synge (1972, chapter VI, § 14).

Charged Particles and Electromagnetic Fields

A charged particle in $\mathcal{M}$ is a triple (α, m, q), where (α, m) is a material particle and q is a nonzero real number called the charge of the particle. Charged particles do two things of interest to us. By their very presence they create electromagnetic fields and they also respond to the electromagnetic fields created by other charges.

Charged particles "respond" to an electromagnetic field by experiencing changes in 4-momentum. The quantitative nature of this response, that is, the equation of motion, is generally taken to be the so-called Lorentz 4-force law which expresses the proper time rate of change of the particle's 4-momentum at each point of the world line as a linear function of the 4-velocity. Thus, at each point $\alpha(\tau)$ of the world line

$$\frac{dP(\tau)}{d\tau} = q\tilde{F}_{\alpha(\tau)}(U(\tau)) \qquad [24]$$

where $\tilde{F}_{\alpha(\tau)}: \mathcal{M} \to \mathcal{M}$ is a linear transformation determined, in each admissible coordinate system, by the classical electric $\boldsymbol{E}$ and magnetic $\boldsymbol{B}$ fields (here we are assuming that the contribution of q to the ambient electromagnetic field is negligible, that is, (α, m, q) is a "test charge"). Let us write [24] more simply as

$$\tilde{F}(U) = \frac{m}{q}\frac{dU}{d\tau} \qquad [25]$$

Dotting both sides of [25] with U gives

$$\tilde{F}(U) \cdot U = \frac{m}{q}\frac{dU}{d\tau} \cdot U = \frac{m}{2q}\frac{d}{d\tau}(U \cdot U)$$
$$= \frac{m}{2q}\frac{d}{d\tau}(-1) = 0$$

Since any future-directed timelike unit vector u is the 4-velocity of some charged particle, we find that $\tilde{F}(u) \cdot u = 0$ for any such vector. Linearity then implies $\tilde{F}(v) \cdot v = 0$ for any timelike vector. Now, if u and v are timelike and future directed, then $u + v$ is timelike so $0 = \tilde{F}(u + v) \cdot (u + v) = \tilde{F}(u) \cdot v + u \cdot \tilde{F}(v)$ and therefore $\tilde{F}(u) \cdot v = -u \cdot \tilde{F}(v)$. But $\mathcal{M}$ has a basis of future-directed timelike vectors so

$$\tilde{F}(x) \cdot y = -x \cdot \tilde{F}(y) \qquad [26]$$

for all $x, y \in \mathcal{M}$. Thus, at each point, the linear transformation $\tilde{F}$ must be skew-symmetric with respect to the Lorentz inner product. One could therefore model an electromagnetic field on $\mathcal{M}$ by an assignment to each point of a skew-symmetric linear transformation whose job it is to assign to the 4-velocity of a charged particle whose world line passes through that point the change in 4-momentum that the particle should expect to experience because of the presence of the field. However, a slightly different perspective has proved more convenient. Notice that a skew-symmetric linear transformation $\tilde{F}: \mathcal{M} \to \mathcal{M}$ and the Lorentz inner product together determine a bilinear form $F: \mathcal{M} \times \mathcal{M} \to \mathbb{R}$ given by

$$F(x, y) = \tilde{F}(x) \cdot y$$

which is also skew-symmetric ($F(y, x) = \tilde{F}(y) \cdot x = -F(x, y)$) and that, conversely, a skew-symmetric bilinear form uniquely determines a skew-symmetric linear transformation. Now, an assignment of a skew-symmetric bilinear form to each point of $\mathcal{M}$ is nothing other than a 2-form on $\mathcal{M}$ and it is in the language of forms that we choose to phrase classical electromagnetic theory (a concise introduction to this language is available, for example, in Spivak (1965, chapter 4).

Nature imposes a certain restriction on which 2-forms can reasonably represent an electromagnetic field on $\mathcal{M}$ ("Maxwell's equations"). To formulate these we introduce a source 1-form J as follows: If

x^1, x^2, x^3, x^4 is any admissible coordinate system on $\mathcal{M}$, then

$$J = J_1 dx^1 + J_2 dx^2 + J_3 dx^3 - \rho dx^4 \qquad [27]$$

where $\rho: \mathcal{M} \to \mathbb{R}$ is a charge density function and $\boldsymbol{J} = J_1 e_1 + J_2 e_2 + J_3 e_3$ is a current density vector field (these are to be regarded as the usual "smoothed out," pointwise versions of "charge per unit volume" and "charge flow per unit area per unit time" as measured by the corresponding admissible observer). Now, our formal definition is as follows: The electromagnetic field on $\mathcal{M}$ determined by the source 1-form J on $\mathcal{M}$ is a 2-form F on $\mathcal{M}$ that satisfies Maxwell's equation

$$dF = 0 \qquad [28]$$

and

$$^*d^*F = J \qquad [29]$$

A few comments are in order here. We have chosen units in which not only the speed of light, but also various other constants that one often finds in Maxwell's equations (the dielectric constant ϵ_0 and magnetic permeability μ_0) are 1 and a factor of 4π in [29] is "normalized out." The * in [29] is the Hodge star operator determined by the Lorentz inner product and the chosen orientation of $\mathcal{M}$. This is a natural isomorphism

$$^*: \Omega^p(\mathcal{M}) \to \Omega^{4-p}(\mathcal{M}), \quad p = 0, 1, 2, 3, 4$$

of the p-forms on $\mathcal{M}$ to the $(4-p)$-forms on $\mathcal{M}$ and is most simply defined as follows: let x^1, x^2, x^3, x^4 be any admissible coordinate system on $\mathcal{M}$. If $1 \in \Omega^0(\mathcal{M})$ is the constant function (0-form) on $\mathcal{M}$ whose value is $1 \in \mathbb{R}$, then

$$^*1 = dx^1 \wedge dx^2 \wedge dx^3 \wedge dx^4$$

is the volume form on $\mathcal{M}$. If $1 \leq i_1 < \cdots < i_k \leq 4$, then $^*(dx^{i_1} \wedge \cdots \wedge dx^{i_k})$ is uniquely determined by

$$(dx^{i_1} \wedge \cdots \wedge dx^{i_k}) \wedge {}^*(dx^{i_1} \wedge \cdots \wedge dx^{i_k}) = -dx^1 \wedge dx^2 \wedge dx^3 \wedge dx^4$$

Thus, for example, $^*dx^2 = dx^1 \wedge dx^3 \wedge dx^4$, $^*(dx^1 \wedge dx^2) = -dx^3 \wedge dx^4$, $^*(dx^1 \wedge dx^2 \wedge dx^3 \wedge dx^4) = -1$, etc. It follows that, if μ is a p-form on $\mathcal{M}$, then

$$^{**}\mu = (-1)^{p+1}\mu \qquad [30]$$

(a more thorough discussion is available in Choquet-Bruhat *et al.* (1977, chapter V A3)). In particular, [29] is equivalent to

$$d^*F = {}^*J \qquad [31]$$

On regions in which there are no charges, so that $J = 0$, [28] and [31] become the source free Maxwell equations

$$dF = 0 \qquad [32]$$

and

$$d^*F = 0 \qquad [33]$$

that is, both F and $^*F$ are closed 2-forms.

Any 2-form F on $\mathcal{M}$ can be written in any admissible coordinate system as $F = (1/2)F_{ab}dx^a \wedge dx^b$ (summation convention!), where (F_{ab}) is the skew-symmetric matrix of components of F. In order to make contact with the notation generally employed in physics, we introduce the following names for these components:

$$(F_{ab}) = \begin{pmatrix} 0 & B^3 & -B^2 & E^1 \\ -B^3 & 0 & B^1 & E^2 \\ B^2 & -B^1 & 0 & E^3 \\ -E^1 & -E^2 & -E^3 & 0 \end{pmatrix} \qquad [34]$$

Thus,

$$\begin{aligned} F = {} & E^1 dx^1 \wedge dx^4 + E^2 dx^2 \wedge dx^4 \\ & + E^3 dx^3 \wedge dx^4 + B^3 dx^1 \wedge dx^2 \\ & + B^2 dx^3 \wedge dx^1 + B^1 dx^2 \wedge dx^3 \end{aligned} \qquad [35]$$

Computing $^*F, dF, d^*F$ and $^*d^*F$ and writing $\boldsymbol{E} = E^1 e_1 + E^2 e_2 + E^3 e_3$ and $\boldsymbol{B} = B^1 e_1 + B^2 e_2 + B^3 e_3$ one finds that $dF = 0$ is equivalent to

$$\operatorname{div} \boldsymbol{B} = 0 \qquad [36]$$

and

$$\operatorname{curl} \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = 0 \qquad [37]$$

while $^*d^*F = J$ is equivalent to

$$\operatorname{div} \boldsymbol{E} = \rho \qquad [38]$$

and

$$\operatorname{curl} \boldsymbol{B} - \frac{\partial \boldsymbol{E}}{\partial t} = \boldsymbol{J} \qquad [39]$$

Equations [36]–[39] are the more traditional renderings of Maxwell's equations.

In another admissible coordinate system $\hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{x}^4$ on $\mathcal{M}$ (related to the first by [2]) the 2-form F would be written $F = (1/2)\hat{F}_{ab}d\hat{x}^a \wedge d\hat{x}^b$. Setting $\hat{x}^a = \Lambda^a{}_\alpha x^\alpha$ and $\hat{x}^b = \Lambda^b{}_\beta x^\beta$ gives $F = (1/2)(\Lambda^a{}_\alpha \Lambda^b{}_\beta \hat{F}_{ab})dx^\alpha \wedge dx^\beta$, so

$$F_{\alpha\beta} = \Lambda^a{}_\alpha \Lambda^b{}_\beta \hat{F}_{ab}, \quad \alpha, \beta = 1, 2, 3, 4 \qquad [40]$$

Now, suppose that we wish to describe the electromagnetic field of a uniformly moving charge. According to the relativity principle, it does not matter at all whether we view the charge as moving

relative to a "fixed" admissible observer, or the observer as moving relative to a "stationary" charge. Thus, we shall write out the field due to a charge fixed at the origin of the hatted coordinate system ("Coulomb's law") and transform, by [40], to an unhatted coordinate system moving relative to it. Relative to $\hat{x}^1, \hat{x}^2, \hat{x}^3, \hat{x}^4$, the familiar inverse square law for a fixed point charge q located at the spatial origin gives $\hat{B} = 0$ and $\hat{E} = (q/\hat{r}^3)\hat{r}$, where $\hat{r} = \hat{x}^1\hat{e}_1 + \hat{x}^2\hat{e}_2 + \hat{x}^3\hat{e}_3$ and $\hat{r} = ((\hat{x}^1)^2 + (\hat{x}^2)^2 + (\hat{x}^3)^2)^{1/2}$ (note that $\hat{E}$ is defined only on $\mathcal{M} - \text{Span}\{\hat{e}_4\}$). Thus,

$$(\hat{F}_{ab}) = \frac{q}{\hat{r}^3}\begin{pmatrix} 0 & 0 & 0 & \hat{x}^1 \\ 0 & 0 & 0 & \hat{x}^2 \\ 0 & 0 & 0 & \hat{x}^3 \\ -\hat{x}^1 & -\hat{x}^2 & -\hat{x}^3 & 0 \end{pmatrix} \qquad [41]$$

It is a simple matter to verify that, on its domain, $(\hat{F}_{ab})$ satisfies the source free Maxwell equations. Taking Λ to be the special Lorentz transformation corresponding to [5] and writing out [40] with $(\hat{F}_{ab})$ given by [41] yields

$$\begin{aligned} E^1 &= q\left(\frac{\hat{x}^1}{\hat{r}^3}\right) \\ E^2 &= \frac{q}{\sqrt{1-\beta^2}}\left(\frac{\hat{x}^2}{\hat{r}^3}\right) \\ E^3 &= \frac{q}{\sqrt{1-\beta^2}}\left(\frac{\hat{x}^3}{\hat{r}^3}\right) \qquad [42] \\ B^1 &= 0 \\ B^2 &= \frac{-q\beta}{\sqrt{1-\beta^2}}\left(\frac{\hat{x}^3}{\hat{r}^3}\right) \\ B^3 &= \frac{q\beta}{\sqrt{1-\beta^2}}\left(\frac{\hat{x}^2}{\hat{r}^3}\right) \end{aligned}$$

We wish to express these in terms of measurements made by the unhatted observer at the instant the charge passes through his spatial origin. Setting $x^4 = 0$ in [5] gives

$$\hat{x}^1 = \frac{1}{\sqrt{1-\beta^2}}x^1, \quad \hat{x}^2 = x^2, \quad \hat{x}^3 = x^3$$

and so

$$\hat{r}^2 = \frac{1}{1-\beta^2}(x^1)^2 + (x^2)^2 + (x^3)^2$$

which, for convenience, we write r_β^2. Making these substitutions in [42] gives

$$\begin{aligned} \boldsymbol{E} &= \frac{q}{\sqrt{1-\beta^2}}\left(\frac{1}{r_\beta^3}\right)(x^1e_1 + x^2e_2 + x^3e_3) \\ &= \frac{q}{\sqrt{1-\beta^2}}\left(\frac{1}{r_\beta^3}\right)\boldsymbol{r} \qquad [43] \end{aligned}$$

and

$$\begin{aligned} \boldsymbol{B} &= \frac{q}{\sqrt{1-\beta^2}}\left(\frac{1}{r_\beta^3}\right)(0e_1 - \beta x^3e_2 + \beta x^2e_3) \\ &= \frac{q}{\sqrt{1-\beta^2}}\left(\frac{1}{r_\beta^3}\right)((\beta e_1) \times \boldsymbol{r}) \qquad [44] \end{aligned}$$

for the field of a charge moving uniformly with velocity βe_1 at the instant the charge passes through the origin. Observe that when $\beta \ll 1, r_\beta \approx r$, so [43] says that the electric field of a slowly moving charge is approximately the Coulomb field. When $\beta \ll 1$, [44] reduces to the Biot–Savart law.

Let us consider one other simple application, that is, the response of a charged particle (α, m, q) to an electromagnetic field which, for some admissible observer, is constant and purely magnetic. For simplicity, we assume that, for this observer $\boldsymbol{E} = 0$ and $\boldsymbol{B} = be_3$, where b is a nonzero constant. The corresponding 2-form F has components

$$(F_{ab}) = \begin{pmatrix} 0 & b & 0 & 0 \\ -b & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

(from [34]). The corresponding linear transformation $\tilde{F}$ has the same matrix relative to this basis so, with $\alpha(\tau) = x^a(\tau)e_a$ and $U(\tau) = U^a(\tau)e_a$, the Lorentz 4-force law [25] reduces to the system of linear differential equations

$$\begin{aligned} \frac{dU^1}{d\tau} &= \frac{bq}{m}U^2, & \frac{dU^2}{d\tau} &= -\frac{bq}{m}U^1 \\ \frac{dU^3}{d\tau} &= 0, & \frac{dU^4}{d\tau} &= 0 \end{aligned}$$

The system is easily solved and the results easily integrated to give

$$\begin{aligned} \alpha(\tau) = x_0 &+ a\sin\left(\frac{bq\tau}{m} + \phi\right)e_1 \\ &+ a\cos\left(\frac{bq\tau}{m} + \phi\right)e_2 \\ &+ c\tau e_3 + \left(1 + \frac{a^2b^2q^2}{m^2} + c^2\right)\tau e_4 \qquad [45] \end{aligned}$$

where $x_0 = x_0^a e_a \in \mathcal{M}$ is constant and a, ϕ, and c are real constants with $a > 0$ (we have used $U \cdot U = -1$ to eliminate one other arbitrary real constant). Note that, at each point on α, $(x^1 - x_0^1)^2 + (x^2 - x_0^2)^2 = a^2$. Thus, if $c \neq 0$ the spatial trajectory in this coordinate system is a helix along the e_3-direction (i.e., along the magnetic field lines). If $c = 0$, the trajectory is a circle in the x^1–x^2 plane. This case is of some practical significance since one can

introduce constant magnetic fields in a bubble chamber so as to induce a particle of interest to follow a circular path. We show now how to measure the charge-to-mass ratio for such a particle. Taking $c=0$ in [45] and computing $U(\tau)$, then using [11] to solve for the coordinate velocity vector V of the particle gives

$$V=\frac{abq/m}{\sqrt{1-\|V\|^2}}\left(\cos\left(\frac{bq\tau}{m}+\phi\right)e_1 + \sin\left(\frac{bq\tau}{m}+\phi\right)e_2\right)$$

From this one computes

$$\|V\|^2=\left(1+\frac{m^2}{a^2b^2q^2}\right)^{-1}$$

(note that this is a constant). Solving this last equation for q/m (and assuming $q>0$ for convenience) one arrives at

$$\frac{q}{m}=\frac{1}{a|b|}\frac{\|V\|}{\sqrt{1-\|V\|^2}}$$

Since a, b, and $\|V\|$ are measurable, one obtains the desired charge-to-mass ratio.

To conclude we wish to briefly consider the existence and use of "potentials" for electromagnetic fields. Suppose F is an electromagnetic field defined on some connected, open region X in $\mathcal{M}$. Then F is a 2-form on X which, by [28], is closed. Suppose also that the second de Rham cohomology $H^2(X;\mathbb{R})$ of X is trivial (since $\mathcal{M}$ is topologically $\mathbb{R}^4$ this will be the case, for example, when X is all of $\mathcal{M}$, or an open ball in $\mathcal{M}$, or, more generally, an open "star-shaped" region in $\mathcal{M}$). Then, by definition, every closed 2-form on X is exact so, in particular, there exists a 1-form A on X satisfying

$$F=\mathrm{d}A \qquad [46]$$

In particular, such a 1-form A always exists locally on a neighborhood of any point in X for any F. Such an A is not uniquely determined, however, because, if A satisfies [46], then so does $A+\mathrm{d}f$ for any smooth real-valued function (0-form) f on X ($\mathrm{d}^2=0$ implies $\mathrm{d}(A+\mathrm{d}f)=\mathrm{d}A+\mathrm{d}^2f=\mathrm{d}A=F$). Any 1-form A satisfying [46] is called a (gauge) potential for F. The replacement $A\to A+\mathrm{d}f$ for some f is called a gauge transformation of the potential and the freedom to make such a replacement without altering [46] is called gauge freedom.

One can show that, given F, it is always possible to locally solve $\mathrm{d}A=F$ for A subject to an arbitrary specification of the 0-form ${}^*\mathrm{d}^*A$. More precisely, if F is any 2-form satisfying $\mathrm{d}F=0$ and g is an arbitrary 0-form, then locally, on a neighborhood of any point, there exists a 1-form A satisfying

$$\mathrm{d}A=F \quad \text{and} \quad {}^*\mathrm{d}^*A=g \qquad [47]$$

(a more general result is proved in Parrott (1987, appendix 2) and a still more general one in section 2.9 of this same source). The usefulness of the second condition in [47] can be illustrated as follows. Suppose we are given some (physical) configuration of charges and currents (i.e., some source 1-form J) and we wish to find the corresponding electromagnetic field F. We must solve Maxwell's equations $\mathrm{d}F=0$ and ${}^*\mathrm{d}^*F=J$ (subject to whatever boundary conditions are appropriate). Locally, at least, we may seek instead a corresponding potential A (so that $F=\mathrm{d}A$). Then the first of Maxwell's equations is automatically satisfied ($\mathrm{d}F=\mathrm{d}(\mathrm{d}A)=0$) and we need only solve ${}^*\mathrm{d}^*(\mathrm{d}A)=J$. To simplify the notation let us temporarily write $\delta={}^*\mathrm{d}^*$ and consider the operator $\Delta=\mathrm{d}\circ\delta+\delta\circ\mathrm{d}$ on forms (variously called the Laplace–Beltrami operator, Laplace–de Rham operator, or Hodge Laplacian on Minkowski spacetime). Then

$$\Delta A=\mathrm{d}(\delta A)+\delta(\mathrm{d}A)=\mathrm{d}({}^*\mathrm{d}^*A)+{}^*\mathrm{d}^*(\mathrm{d}A) \qquad [48]$$

According to the result quoted above, we may narrow down our search by imposing the condition ${}^*\mathrm{d}^*A=0$, that is

$$\delta A=0 \qquad [49]$$

(this is generally referred to as imposing the Lorentz gauge). With this, [48] becomes $\Delta A={}^*\mathrm{d}^*(\mathrm{d}A)$ and to satisfy the second Maxwell equation we must solve

$$\Delta A=J \qquad [50]$$

Thus, we see that the problem of (locally) solving Maxwell's equations for a given source J reduces to that of solving [49] and [50] for the potential A. To understand how this simplifies the problem, we note that a calculation in admissible coordinates shows that the operator Δ reduces to the componentwise d'Alembertian $\Box$, defined on real-valued functions by

$$\Box=\frac{\partial^2}{\partial(x^1)^2}+\frac{\partial^2}{\partial(x^2)^2}+\frac{\partial^2}{\partial(x^3)^2}-\frac{\partial^2}{\partial(x^4)^2}$$

Thus, eqn [50] decouples into four scalar equations

$$\Box A_a=J_a, \quad a=1,2,3,4 \qquad [51]$$

each of which is the well-studied inhomogeneous wave equation.

Further Reading

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Introductory Article: Quantum Mechanics

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Historical Background

In this section we shall briefly recall the basic empirical facts and the first theoretical attempts from which the theory and the formalism of present-day quantum mechanics (QM) has grown. In the next sections we shall give the mathematical and computational structure of QM, mention the physical problems that QM has solved with much success, and describe the serious conceptual consistency problems which are posed by QM (and which remain unsolved up to now).

Empirical rules of discretization were observed already, starting from the 1850s, in the absorption and in the emission of light. Fraunhofer noticed that the dark lines in the absorption spectrum of the light of the sun coincide with the bright lines in the emission lines of all elements. G Kirchhoff and R Bunsen reached the conclusion that the relative intensities of the emission and absorption of light implied that the ratio between energy emitted and absorbed is independent of the atom considered. This was the starting point of the analysis by Planck.

On the other hand, by the end of the eighteenth century, the spatial structure of the atom had been investigated; the most successful model was that of Rutherford, in which the atom appeared as a small nucleus of charge Z surrounded by Z electrons attracted by the nucleus according to Coulomb's law. This model represents, for distances of the order of the size of an atom, a complete departure from Newton's laws combined with the laws of classical electrodynamics; indeed, according to these laws, the atom would be unstable against collapse, and would certainly not exhibit a discrete energy spectrum. We must conclude that the classical laws are inadequate for the description of emission and absorption of light, in which the internal structure of the atom plays a major role.

The birth of the old quantum theory is placed traditionally at the date of M Planck's discussion of the blackbody radiation in 1900.

Planck put forward the postulate that light is emitted and absorbed by matter in discrete energy quanta through "resonators" that have an energy proportional to their frequency. This assumption led, through the use of Gibb's rules of Statistical Mechanics applied to a gas of resonators, to a law (Planck's law) which reproduces the empirical findings on the radiation from a blackbody. It led Einstein to ascribe to light (which had, since the times of Maxwell, a successful description in terms of waves) a discrete, particle-like nature. Nine years later A Einstein gave further support to Planck's postulate by showing that it can reproduce correctly the energy fluctuations in blackbody radiation and even clarifies the properties of specific heat. Soon afterwards, Einstein (1924, 1925) proved that the putative particle of light satisfied the relativistic laws (relation between energy and momentum) of a particle with zero mass.

This dual nature of light received further support from the experiments on the Compton effect and from description, by Einstein, of the photoelectric effect (Einstein 1905). It should be emphasized that while Planck considered with light in interaction with matter ν as composed of bits of energy $h\nu$ ($h \simeq 6,6 \times 10^{-27}$ erg s), Einstein's analysis went much further in assigning to the quantum of light properties of a particle-like (localized) object. This marks a complete departure from the laws of classical electromagnetism. Therefore, quoting Einstein,

> It is conceivable that the wave theory of light, which retains its effectiveness for the representation of purely optical phenomena and is based on continuous functions over space, will lead to contradiction with the experiments when applied to phenomena in which there is creation or conversion of light; indeed these phenomena can be better

> described on the assumption that light is distributed discontinuously in space and described by a finite number of quanta which move without being divided and which must be absorbed or emitted as a whole.

Notice that, for wavelength of 8×10^3 Å, a 30 W lamp emits roughly 10^{20} photons s^{-1}; for macroscopic objects the discrete nature of light has no appreciable consequence.

Planck's postulate and energy conservation imply that in emitting and absorbing light the atoms of the various elements can lose or gain energy only by discrete amounts. Therefore, atoms as producers or absorbers of radiation are better described by a theory that assigns to each atom a (possible infinite) discrete set of states which have a definite energy.

The old quantum theory of matter addresses precisely this question. Its main proponent is N Bohr (Bohr 1913, 1918). The new theory is entirely phenomenological (as is Planck's theory) and based on Rutherford's model and on three more postulates (Born 1924):

(i) The states of the atom are stable periodic orbits, as given by Newton's laws, of energy $E_n, n \in Z^+$, given by $E_n = h\nu_n f(n)$, where h is Plank's constant, ν_n is the frequency of the electron on that orbit, and $f(n)$ is for each atom a function approximately linear in Z at least for small values of Z.

(ii) When radiation is emitted or absorbed, the atom makes a transition to a different state. The frequency of the radiation emitted or absorbed when making a transition is $\nu_{n,m} = h^{-1}|E_n - E_m|$.

(iii) For large values of n and m and small values of $(n-m)/(n+m)$ the prediction of the theory should agree with those of the classical theory of the interaction of matter with radiation.

Later, A Sommerfeld gave a different version of the first postulate, by requiring that the allowed orbits be those for which the classical action is an integer multiple of Planck's constant.

The old quantum theory met success when applied to simple systems (atoms with $Z < 5$) but it soon appeared evident that a new, radically different point of view was needed and a fresh start; the new theory was to contain few free parameters, and the role of postulate (iii) was now to fix the value of these parameters.

There were two (successful) attempts to construct a consistent theory; both required a more sharply defined mathematical formalism. The first one was sparked by W Heisenberg, and further important ideas and mathematical support came from M Born, P Jordan, W Pauli, P Dirac and, on the mathematical side, also by J von Neumann and A Weyl. This formulation maintains that one should only consider relations between observable quantities, described by elements that depend only on the initial and final states of the system; each state has an internal energy. By energy conservation, the difference between the energies must be proportional (with a universal constant) to the frequency of the radiation absorbed or emitted. This is enough to define the energy of the state of a single atom modulo an additive constant. The theory must also take into account the probability of transitions under the influence of an external electromagnetic field.

We shall give some details later on, which will help to follow the basis of this approach.

The other attempt was originated by L de Broglie following early remarks by HW Bragg and M Brillouin. Instead of emphasizing the discrete nature of light, he stressed the possible wave nature of particles, using as a guide the Hamilton–Jacobi formulation of classical mechanics. This attempt was soon supported by the experiments of Davisson and Germer (1927) of scattering of a beam of ions from a crystal. These experiments showed that, while electrons are recorded as "point particles," their distribution follows the law of the intensity for the diffraction of a (dispersive) wave. Moreover, the relation between momentum and frequency was, within experimental errors, the same as that obtained by Einstein for photons.

The theory started by de Broglie was soon placed in almost definitive form by E Schrödinger. In this approach one is naturally led to formulate and solve partial differential equations and the full development of the theory requires regularity results from the theory of functions.

Schrödinger soon realized that the relations which were found in the approach of Heisenberg could be easily (modulo technical details which we shall discuss later) obtained within the formalism he was advocating and indeed he gave a proof that the two formalisms were equivalent. This proof was later refined, from the mathematical point of view, by J von Neumann and G Mackey.

In fact, Schrödinger's approach has proved much more useful in the solution of most physical problems in the nonrelativistic domain, because it can rely on the developments and practical use of the theory of functions and of partial differential equations. Heisenberg's "algebraic" approach has therefore a lesser role in solving concrete problems in (nonrelativistic) QM.

If one considers processes in which the number of particles may change in time, one is forced to

introduce a Hilbert space that accommodates states with an arbitrarily large number of particles, as is the case of the theory of relativistic quantized field or in quantum statistical mechanics; it is then more difficult to follow the line of Schrödinger, due to difficulties in handling spaces of functions of infinitely many variables. The approach of Heisenberg, based on the algebra of matrices, has a rather natural extension to suitable algebras of operators; the approach of Schrödinger, based on the description of a state as a (wave) function, encounters more difficulties since one must introduce functionals over spaces of functions and the description of dynamics does not have a simple form.

From this point of view, the generalization of Heisenberg's approach has led to much progress in the understanding of the structure of the resulting theory. Still some relevant results have been obtained in a Schrödinger representation. We shall not elaborate further on this point.

We shall end this introductory section with a short description of the emergence of the structure of QM in Heisenberg's and Schrödinger's approaches; this will provide a motivation for the axiom of QM which we shall introduce in the following section. For an extended analysis, see, for example, Jammer (1979).

The specific form that was postulated by de Broglie (1923) for the wave nature of a particle relies on the relation of geometrical optics with wave propagation and on the formulation of Hamiltonian mechanics as a sort of "wave front propagation" through the solution of the Hamilton–Jacobi equation and the introduction of group velocity.

By the analogy with electromagnetic wave, it is natural to associate with a free nonrelativistic particle of momentum p and mass m the plane wave

$$\phi_p(x,t) = e^{i(px-Ft)/\hbar}, \quad \hbar = \frac{h}{2\pi}, \quad E = \frac{p^2}{2m}$$

Schrödinger obtained the equation for a quantum particle in a field of conservative forces with potential $V(x)$ by considering an analogy with the propagation of an electromagnetic wave in a medium with refraction index $n(x,\omega)$ that varies slowly on the scale of the wavelength. Indeed, in this case the "wave" follows the laws of geometrical optics, and has therefore a "particle-like" behavior. If one denotes by $\hat{u}(x,\omega)$ the Fourier transom (with respect to time) of a generic component of the electric field and one assumes that the field be essentially monochromatic (so that the support of $\hat{u}(x,\omega)$ as a function of ω is in a very small neighborhood of ω_0), one finds that $\hat{u}(x,\omega)$ is an approximate solution of the equation

$$-\Delta\hat{u}(x,\omega) = \frac{\omega_0^2}{c^2} n^2(x,\omega)\hat{u}(x,\omega) \qquad [1]$$

Writing $u(x,\omega) = A(x,\omega)\, e^{i(\omega/c)W(x,\omega)}$ the phase $W(x,\omega)$ satisfies, in the high-frequency limit, the eikonal equation $|\nabla W(x,\omega)|^2 = n^2(x,\omega)$. One can define for the solution a *phase velocity* v_f and it turns out that $v_f = c/|\nabla W(x,\omega)|$.

On the other hand, classical mechanics can also be described by propagation of surfaces of constant value for the solution $W(x,\ t)$ of the Hamilton–Jacobi equation $H(x, \nabla W) = E$, with $H = p^2/2m + V(x)$. Recall that high-frequency (the realm of geometric optics) corresponds to small distances. This analogy led Schrödinger (1926) to postulate that the dynamics satisfied by the waves associated with the particles was given by the (Schrödinger) equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta_x\psi(x,t) + V(x)\psi(x,t) \qquad [2]$$

This wave was to describe the particle and its motion, but, being complex valued, it could not represent any measurable property. It is a mathematical property of the solutions of [2] that the quantity $\int |\psi(x,t)|^2\, d^3x$ is preserved in time. Furthermore, if one sets

$$\rho(x,t) \equiv |\psi(x,t)|^2$$

$$j(x,t) \equiv -i\frac{\hbar}{2m}[\bar{\psi}(x,t)\nabla\psi(x,t) - \psi(x,t)\nabla\bar{\psi}(x,t)] \qquad [3]$$

one easily verifies the local conservation law

$$\frac{\partial\rho}{\partial t} + \text{div}\ j(x,t) = 0 \qquad [4]$$

These mathematical properties led to the statistical interpretation given by Max Born: in those experiments in which the position of the particles is measured, the integral of $|\psi(x,t)|^2$ over a region Ω of space gives the probability that at time t the particle is localized in the region Ω. Moreover, the current associated with a charged particle is given locally by $j(x,t)$ defined above.

Let us now briefly review Heisenberg's approach. At the heart of this approach are: empirical formulas for the intensities of emission and absorption of radiation (dispersion relations), Sommerfeld's quantum condition for the action and the vague statement "the analogue of the derivative for the discrete action variable is the corresponding finite difference quotient." And, most important, the remark that the correct description of atomic physics was through quantities associated with pairs of states, that is, (infinite) matrices and the

empirical fact that the frequency (or rather the wave number) $\omega_{k,j}$ of the radiation (emitted or absorbed) in the transition between the atomic levels k and j ($k \neq j$) satisfies the Ritz combination principle $\omega_{m,j} + \omega_{j,k} = \omega_{m,k}$. It easy to see that any doubly indexed family satisfying this relation must have the form $\omega_{m,k} = E_m - E_k$ for suitable constant E_j.

It was empirically verified by Kramers that the dipole moment of an atom in an external monochromatic external field with frequency ν was proportional to the field with a coefficient (of polarization)

$$P - \frac{e^2}{4\pi m} \sum_i \left[\frac{f_i}{\nu_i^2 - \nu^2} - \frac{F_i}{\nu_i^2 - \nu^2} \right] \qquad [5]$$

where e, m are the charge and the mass of the electron and f_i, F_i are the probabilities that the frequency ν is emitted or absorbed.

A detailed analysis of the phenomenon of polarization in classical mechanics, with the clearly stated aim "of presenting the results in a way that may give hints for the construction of a New Mechanics" was made by Max Born (1924). He makes use of action-angle variables $\{J_i, \theta_i\}$ assuming that the atom can be considered as a collection of harmonic oscillators with frequency ν_i coupled linearly to the electric field of frequency μ.

In the dipole approximation one obtains the following result for the polarization P (linear response in energy to the electric field):

$$P = - \sum_{(\nu \cdot m) > 0} 2(m \cdot \nabla_J) \frac{|A(J)|^2 (\nu \cdot m)}{((m \cdot \nu)^2 - \mu} \qquad [6]$$

where $\nu_k = \partial H / \partial J_k$, H is the interaction Hamiltonian), and $A(J)$ is a suitable matrix. In order to derive the new dynamics, having as a guide the correspondence principle, one has to compare this result with the Kramers dispersion relation, which we write (to make the comparison easier) in the form

$$P = \frac{e^2}{4\pi m} \sum_{n,m} \frac{f_{m,n}}{\nu_{n,m}^2 - \mu^2} - \frac{f_{n,m}}{\nu_{n,m}^2 - \mu^2} \quad E_m > E_n \qquad [7]$$

Bohr's rule implies that $\nu(n + \tau, n) = (E(n + \tau - E(n))/\hbar$.

Born and Heisenberg noticed that, for n sufficiently large and k small, one can approximate the differential operator in [6] with the corresponding difference operator, with an error of the order of k/n. Therefore, [6] could be substituted by

$$P = -\hbar^{-1} \sum_{m_k > 0} \left[\frac{|A_{n+m,n}|^2}{\nu(n+m)^2 - \mu^2} - \frac{|A_{n-m,n}|^2}{\nu(n-m)^2 - \mu^2} \right] \qquad [8]$$

The conclusion Born and Heisenberg drew is that the matrix A that takes the place of the momentum in the classical theory must be such that $|A_{n+m,n}|^2 = e^2 \hbar m^{-1} f(n+m, n)$. In the same vein, considering the polarization in a static electric field, it is possible to find an expression for the matrix that takes the place of the coordinate x in classical Hamiltonian theory.

In general, the new approach (matrix mechanics) associates matrices with some relevant classical observables (such as functions of position or momentum) with a time dependence that is derived from the empirical dispersion relations of Kramers, the correspondence principle, Bohr's rule, Sommerfeld action principle and first- (and second-) order perturbation theory for the interaction of an atom with an external electromagnetic field. It was soon clear to Born and Jordan (1925) that this dynamics took the form $i\hbar \dot{A} = AH - HA$ for a matrix H that for the case of the hydrogen atom is obtained for the classical Hamiltonian with the prescription given for the coordinates x and p. It was also seen as plausible the relation $[\hat{x}_j, \hat{p}_k] = \mathrm{i}I$ among the matrices $\hat{x}_k$ and $\hat{p}_k$ corresponding to position and momentum. One year later P Dirac (1926) pointed out the structural identity of this relation with the Poisson bracket of Hamiltonian dynamics, developed a "quantum algebra" and a "quantum differentiation" and proved that any *-derivation δ (derivation which preserves the adjoint) of the algebra $\mathcal{B}_N$ of $N \times N$ matrices is inner, that is, is given by $\delta(a) = \mathrm{i}[a, h]$ for a Hermitian matrix h. Much later this theorem was extended (with some assumptions) to the algebra of all bounded operators on a separable Hilbert space. Since the derivations are generators of a one-parameter continuous group of automorphisms, that is, of a dynamics, this result led further strength to the ideas of Born and Heisenberg.

The algebraic structure introduced by Born, Jordan, and Heisenberg (1926) was used by Pauli (1927) to give a purely group-theoretical derivation of the spectrum of the hydrogen atom, following the lines of the derivation in symplectic mechanics of the SO(4) symmetry of the Coulomb system. This remarkable success gave much strength to the Heisenberg formulation of QM, which was soon recognized as an efficient instrument in the study of the atomic world.

The algebraic formulation was also instrumental in the description given by Pauli (1928) of the "spin" (a property of electrons empirically postulated by Goudsmidt and Uhlenbeck to account for a hyperfine splitting of some emission lines) as "internal" degree of freedom without reference to spatial coordinates and still connected with the

properties of the the system under the group of spatial rotations. This description through matrices has a major role also in the formulation by Pauli of the exclusion principle (and its relation with Fermi–Dirac statistics), which gave further credit to the Heisenberg's theory by helping in reproducing correctly the classification of the atoms.

These features may explain why the "standard" formulation of the axioms of QM given in the next section shows the influence of Heisenberg's approach. On the other hand, comparison with experiments is usually set in the framework in Schrödinger's approach. Posing the problems in terms of properties of the solution of the Schrödinger equation, one is led to a pragmatic use of the formalism, leaving aside difficulties of interpretation. This separation of "the axioms" from the "practical use" may be one of the reasons why a serious analysis of the axioms and of the problems that arise from them is apparently not a concern for most of the research in QM, even from the point of view of mathematical physics.

One should stress that both the approach of Born and Heisenberg and that of de Broglie and Schrödinger are rooted in a mixture of attention to the experimental data, deep understanding of the previous theory, bold analogies and approximations, and deep concern for the consistency of the "new mechanics."

There is an essential difference between the starting points of the two approaches. In Heisenberg's approach, the atom has *a priori* no spatial structure; the description is entirely in terms of its properties under emission and absorption of light, and therefore its observable quantities are represented by matrices. Dynamics enters through the study of the interaction with the electromagnetic field, and some analogies with the classical theory of electrodynamics in an asymptotic regime (correspondence principle). In this way, as we have briefly indicated, the special role of some matrices, which have a mutual relation similar to the relation of position and momentum in Hamiltonian theory. Following this analogy, it is possible to extend the theory beyond its original scope and consider phenomena in which the electrons are not bound to an atom.

In the approach of Schrödinger, on the other hand, particles and collections of particles are represented by spatial structures (waves). Spatial coordinates are therefore introduced *a priori*, and the position of a particle is related to the intensity of the corresponding wave (this was stressed by Born). Position and momentum are both basic measurable quantities as in classical mechanics. Physical interpretation forces the particle wave to be square integrable, and mathematics provides a limitation on the simultaneous localization in momentum and position leading to Heisenberg's uncertainty principle. Dynamics is obtained from a particle–wave duality and an analogy with the relativistic wave equation in the low-energy regime. The presence of bound states with quantized energies is seen as a consequence of the well-known fact that waves confined to a bounded spatial region have their wave number (and therefore energy) quantized.

Formal Structure

In this section we describe the formal mathematical structure that is commonly associated with QM. It constitutes a coherent mathematical theory, but the interpretation axiom it contains leads to conceptual difficulties.

We state the axioms in the form in which they were codified by J von Neumann (1966); they constitute a mathematically precise rendering of the formalism of Born, Heisenberg, and Jordan. The formalism of Schrödinger *per se* does not require general statements about the category of observables.

Axiom I

(i) Observables are represented by self-adjoint operators in a complex separable Hilbert space $\mathcal{H}$.
(ii) Every such operator represents an observable.

Remark Axiom I (ii) is introduced only for mathematical simplicity. There is no physical justification for part (ii). In principle, an observable must be connected to a procedure of measurement (observation) and for most of the self-adjoint operators on $\mathcal{H}$ (e.g., in the Schrödinger representation for $ix_k(\partial/\partial x_h)x_k$) such procedure has not yet been given).

Axiom II

(i) Pure states of the systems are represented by normalized vectors in $\mathcal{H}$.
(ii) If a measurement of the observable A is made on a system in the state represented by the element $\phi \in \mathcal{H}$, the average of the numerical values one obtains is $<\phi, A\phi>$, a real number because A is self-adjoint (we have denoted by $<\phi, \psi>$ the scalar product in $\mathcal{H}$).

Remark Notice that Axiom II makes no statement about the outcome of a single measurement.

Using the natural complex structure of $\mathcal{B}(\mathcal{H})$, pure states can be extended as linear real functionals on $\mathcal{B}(\mathcal{H})$.

One defines a state as any linear real positive functional on $\mathcal{B}(\mathcal{H})$ (all bounded operators on the separable Hilbert space $\mathcal{H}$) and says that a state is normal if it is continuous in the strong topology. It can be proved that a normal state can be decomposed into a convex combination of at most a denumerable set of pure states. With these definitions a state is pure iff it has no nontrivial decomposition. It is worth stressing that this statement is true only if the operators that correspond to observable quantities generate all of $\mathcal{B}(\mathcal{H})$; one refers to this condition by stating that there are no superselection rules.

By general results in the theory of the algebra $\mathcal{B}(\mathcal{H})$, a normal state ρ is represented by a positive operator of trace class σ through the formula $\rho(A) = Tr(\sigma A)$. Since a positive trace-class operator (usually referred to as density matrix in analogy with its classical counterpart) has eigenvalues λ_k that are positive and sum up to 1, the decomposition of the normal state ρ takes the form $\sigma = \sum_k \lambda_k \Pi_k$, where Π_k is the projection operator onto the kth eigenstate (counting multiplicity).

It is also convenient to know that if a sequence of normal states σ_k on $\mathcal{B}(\mathcal{H})$ converges weakly (i.e., for each $A \in \mathcal{B}(\mathcal{H})$ the sequence $\sigma_k(A)$ converges) then the limit state is normal. This useful result is false in general for closed subalgebras of $\mathcal{B}(\mathcal{H})$, for example, for algebras that contain no minimal projections.

Note that no pure state is dispersion free with respect to all the observables (contrary to what happens in classical mechanics). Recall that the dispersion of the state ρ_σ with respect to the observable A is defined as $\Delta_\sigma(A) \equiv \sigma(A^2) - (\sigma(A))^2$.

The connection of the state with the outcome of a single measurement of an observable associated with an operator A is given by the following axiom, which we shall formulate only for the case when the self-adjoint operator A has only discrete spectrum. The generalization to the other case is straightforward but requires the use of the spectral projections of A.

Axiom III

(i) If A has only discrete spectrum, the possible outcomes of a measurement of A are its eigenvalues $\{a_k\}$.

(ii) If the state of the system immediately before the measurement is represented by the vector $\phi \in \mathcal{H}$, the probability that the outcome be a_k is $\sum_h |<\psi, \phi_h^{A;k}>|$, where $\phi_h^{A;k}$ are a complete orthonormal set in the Hilbert space spanned by the eigenvectors of A to the eigenvalue a_k.

(iii) If a system is in the pure state ϕ and one performs a measurement of the observable A with outcome $a_j \in (b-\delta, b+\delta)$ for some $b, \delta \in R$ then immediately after the measurement the system can be in any (not necessarily pure) state which lies in the convex hull of the pure states which are in the spectral subspace of the operator A in the interval $\Delta_{b;\delta} \equiv (b-\delta, b+\delta)$.

Note Statements (ii) and (iii) can be extended without modification to the case in which the initial state is not a pure state, and is represented by a density matrix σ.

Remark 1 Axiom III makes sure that if one performs, immediately after the first, a further measurement of the same observable A the outcome will still lie in the interval $\Delta_{b;\delta}$. This is needed to give some objectivity to the statement made about the outcome; notice that one must place the condition "immediately after" because the evolution may not leave invariant the spectral subspaces of A. If the operator A has, in the interval $\Delta_{b;\delta}$, only discrete (pure point) spectrum, one can express Axiom III in the following way: the outcome can be any state that can be represented by a convex affine superposition of the eigenstates of A with eigenvalues contained in $\Delta_{b;\delta}$.

In the very special case when A has only one eigenvalue in $\Delta_{b;\delta}$ and this eigenvalue is not degenerate, one can state Axiom III in the following form (commonly referred to as "reduction of the wave packet"): the system after the measurement is pure and is represented by an eigenstate of the operator A.

Remark 2 Notice that the third axiom makes a statement about the state of the system after the measurement is completed.

It follows from Axiom III that one can measure "simultaneously" only observables which are represented by self-adjoint operators that commute with each other (i.e., their spectral projections mutually commute). It follows from the spectral representation of the self-adjoint operators that a family $\{A_k\}$ of commuting operators can be considered (i.e., there is a representation in which they are) functions over a common measure space.

Axioms I–III give a mathematically consistent formulation of QM and allow a statistical description (and statistical prediction) of the outcome of the measurement of any observable. It is worth remarking that while the predictions will have only a statistical nature, the dynamical evolution of the observables (and by duality of the states) will be described by deterministic laws. The intrinsically statistical aspect of the predictions comes only from

the third postulate, which connects the mathematical content of the theory with the measurement process.

The third axiom, while crucial for the connection of the mathematical formalism with the experimental data, contains the seed of the conceptual difficulties which plague QM and have not been cured so far.

Indeed, the third axiom indicates that the process of measurement is described by laws that are intrinsically different from the laws that rule the evolution without measurement. This privileged role of the changing by effect of a measurement leads to serious conceptual difficulties since the changing is independent of whether or not the result is recorded by some observer; one should therefore have a way to distinguish between measurements and generic interactions with the environment.

A related problem that is originated by Axiom III is that the formulation of this axiom refers implicitly to the presence of a classical observer that certifies the outcomes of measurements and is allowed to make use of classical probability theory. This observer is not subjected therefore to the laws of QM.

These two aspects of the conceptual difficulties have their common origin in the separation of the measuring device and of the measured systems into disjoint entities satisfying different laws. The difficulties in the theory of measurement have not yet received a satisfactory answer, but various attempts have been made, with various degree of success, and some of them are described briefly in the section "Interpretation problems." It appears therefore that QM in its present formulation is a refined and successful instrument for the description of the nonrelativistic phenomena at the Planck scale, but its internal consistency is still standing on shaky ground.

Returning to the axioms, it is worth remarking explicitly that according to Axiom II a state is a linear functional over the observables, but it is represented by a sesquilinear function on the complex Hilbert space $\mathcal{H}$. Since Axiom II states that any normalized element of $\mathcal{H}$ represents a state (and elements that differ only by a phase represent the same state) together with ϕ, γ also $\xi \equiv a\phi + b\psi$, $|a|^2 + |b|^2 = 1$ represent a state superposition of ϕ and ψ (superposition principle).

But for an observable A, one has in general $\rho_\xi(A) \neq |a|^2\rho_\phi(A) + |b|^2\rho_\psi(A)$, due to the cross-terms in the scalar product. The superposition principle is one of the characteristic features of QM. The superposition of the two pure states ϕ and ψ has properties completely different from those of a statistical mixture of the same two states, defined by the density matrix $\sigma = |a|^2\Pi_\phi + |b|^2\Pi_\psi$, where we have denoted by Π_ϕ the orthogonal projection onto the normalized vector ϕ. Therefore, the search for these interference terms is one of the means to verify the predictions of QM, and their smallness under given conditions is a sign of quasiclassical behavior of the system under study.

Strictly connected to superposition are entanglement and the partial trace operation. Suppose that one has two systems which when considered separately are described by vectors in two Hilbert spaces $\mathcal{H}_i, i = 1, 2$, and which have observables $A_i \in \mathcal{B}(\mathcal{H}_i)$. When we want to study their mutual interaction, it is natural to describe both of them in the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ and to consider the observables $A_1 \otimes I$ and $I \otimes A_2$.

When the systems interact, the interaction will not in general commute with the projection operator Π_1 onto $\mathcal{H}_1$. Therefore, even if the initial state is of the form $\phi_1 \otimes \phi_2, \phi_i \in \mathcal{H}_i$, the final state (after the interaction) is a vector $\xi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ which cannot be written as $\xi = \zeta_1 \otimes \zeta_2$ with $\zeta_i \in \mathcal{H}_i$. It can be shown, however, that there always exist two orthonormal family vectors $\phi_n \in \mathcal{H}_1$ and $\psi_n \in \mathcal{H}_2$ such that $\xi = \sum c_n \phi_n \otimes \psi_n$ for suitable $c_n \in C$, $\sum |c_n|^2 = 1$ (this decomposition is not unique in general).

Recalling that $\rho_{\phi\otimes\psi}(A_1 \otimes I) = \rho_\phi(A_1)$, one can write

$$\rho_\xi(A_1 \otimes I) = \sum |c_n|^2 \rho_{\zeta_n}(A_1) = \rho_\sigma(A_1)$$
$$\sigma \equiv \sum_n |c_n|^2 \Pi_{\phi_n}$$

The map $\Gamma_2 : \rho_\xi \to \rho_{\sigma_1}$ is called reduction or also conditioning) with respect to $\mathcal{H}_2$; it is also called "partial trace" with respect to $\mathcal{H}_2$. The first notation reflects the analogy with conditioning in classical probability theory.

The map Γ_2 can be extended by linearity to a map from normal states (density matrices) on $\mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ to normal states on $\mathcal{B}(\mathcal{H}_1)$ and gives rise to a positivity-preserving and trace-preserving map.

One can in fact prove (Takesaki 1971) that any conditioning for normal states of a von Neumann algebra $\mathcal{M}$ is completely positive in the sense that it remains positive after tensorization of $\mathcal{M}$ with $\mathcal{B}(\mathcal{K})$, where $\mathcal{K}$ is an arbitrary Hilbert space.

It can also be proved that a partial converse is true, that is, that every completely positive trace-preserving map Φ on normal states of a von Neumann algebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ can be written, for a suitable choice of a larger Hilbert space $\mathcal{K}$ and partial isometries V_k, in the form (Kraus form) $\Phi(a) = \sum_k V_k^* a V_k$.

But it must be remarked that, if $U(t)$ is a one-parameter group of unitary operators on $\mathcal{H}_1 \otimes \mathcal{H}_2$ and σ is a density matrix, the one-parameter family of maps $\Gamma(t) \equiv \sigma \rightarrow \Gamma_2(U(t)\sigma U^*(t))$ does not, in general, have the semigroup property $\Gamma(t+s) = \Gamma(t) \cdot \Gamma(s)$ $s, t > 0$ and therefore there is in general no generator (of a reduced dynamics) associated with it. Only in special cases and under very strong hypothesis and approximations is there a reduced dynamics given by a semigroup (Markov property).

Since entanglement and (nontrivial) conditioning are marks of QM, and on the other side the Markov property described above is typical of conditioning in classical mechanics, it is natural to search for conditions and approximations under which the Markov property is recovered, and more generally under which the coherence properties characteristic of QM are suppressed (decoherence). We shall discuss briefly this problem in the section "Interpretation problems," devoted to the attempts to overcome the serious conceptual difficulties that descend from Axiom III.

It is seen from the remarks and definitions above that normal states (density matrices) play the role that in classical mechanics is attributed to measures over phase space, with the exception that pure states in QM do not correspond to Dirac measures (later on we shall discuss the possibility of describing a quantum-mechanical states with a function (Wigner function) on phase space).

In this correspondence, evaluation of an observable (a measurable function over phase space) over a state (a normalized, positive measure) is related to finding the (Hilbert space) trace of the product of an operator in $\mathcal{B}(\mathcal{H})$ with a density matrix. Notice that the trace operation shares some of the properties of the integral, in particular $\operatorname{tr} AB = \operatorname{tr} BA$ if A is in trace class and $B \in \mathcal{B}(\mathcal{H})$ (cf. $g \in L^1$ and $f \in L^\infty$) and $\operatorname{tr} AB > 0$ if A is a density matrix and B is a positive operator. This suggests to define functions over the density matrices that correspond to quantities which are important in the theory of dynamical systems, in particular the entropy.

This is readily done if the Hilbert space is finite dimensional, and in the infinite-dimensional case if one takes as observables all Hermitian bounded operators. In quantum statistical mechanics one is led to consider an infinite collection of subsystems, each one described with a Hilbert space (finite or infinite dimensional) $\mathcal{H}_i, i = 1, 2, \ldots$, the space of representation is a subspace $\mathcal{K}$ of $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots$, and the observables are a (weakly closed) subalgebra $\mathcal{A}$ of $\mathcal{B}(\mathcal{K})$ (typically constructed as an inductive limit of elements of the form $I \otimes I \cdots \otimes A_k \otimes I \cdots$). In this context one also considers normal states on $\mathcal{A}$ and defines a trace operation, with the properties described above for a trace. Most of the definitions (e.g., of entropy) can be given in this enlarged context, but differences may occur, since in general $\mathcal{A}$ does not contain finite-dimensional projections, and therefore the trace function is not the trace commonly defined in a Hilbert space. We shall not describe further this very interesting and much developed theory, of major relevance in quantum statistical mechanics. For a thorough presentation see Ohya and Petz (1993).

The simplest and most-studied example is the case when each Hilbert space $\mathcal{H}_i$ is a complex two-dimensional space. The resulting system is constructed in analogy with the Ising model of classical statistical mechanics, but in contrast to that system it possesses, for each value of the index i, infinitely many pure states. The corresponding algebra of observables is a closed subalgebra of $(C^2 \times C^2)^{\otimes Z}$ and generically does not contain any finite-dimensional projection.

This model, restricted to the case $(C^2 \times C^2)^K$, K a finite integer, has become popular in the study of quantum information and quantum computation, in which case a normalized element of $\mathcal{H}_i$ is called a q-bit (in analogy with the bits of information in classical information theory). It is clear that the unit sphere in $(C^2 \times C^2)$ contains many more than four points, and this gives much more freedom for operations on the system. This is the basis of quantum computation and quantum information, a very interesting field which has received much attention in recent years.

Quantization and Dynamics

The evolution in nonrelativistic QM is described by the Schrödinger equation in the representation in which for an N-particle system the Hilbert space is $L^2(R^{3N} \otimes C^k$, where C^k is a finite-dimensional space which accounts for the fact that some of the particles may have a spin content.

Apart from (often) inessential parameters, the Schrödinger equation for spin-0 particles can be written typically as

$$i\hbar \frac{\partial \phi}{\partial t} = H\phi$$

$$H \equiv \sum_{k=1}^{N} m_k (i\hbar \nabla_k + A_k)^2 + \sum_{k=1}^{N} V_k(x_k) + \sum_{i \neq k,1}^{N} V_{i,k}(x_i - x_k) \qquad [9]$$

where $\hbar$ is Planck's constant, A_k are vector-valued functions (vector potentials), and V_k and $V_{i,k}$ are scalar-valued function (scalar potentials) on R^3.

If some particles have of spin 1/2, the corresponding kinetic energy term should read $-(i\hbar\sigma\cdot\nabla)^2$, where σ_k, $k=1, 2, 3$, are the Pauli matrices and one must add a term $W(x)$ which is a matrix field with values in $C^k\otimes C^k$ and takes into account the coupling between the spin degrees of freedom. Notice that the local operator $i\sigma\cdot\nabla$ is a "square root" of the Laplacian.

A relativistic extension of the Schrödinger equation for a free particle of mass $m\geq 0$ in dimension 3 was obtained by Dirac in a space of spinor-valued functions $\psi_k(x,t), k=0,1,2,3$, which carries an irreducible representation of the Lorentz group. In analogy with the electromagnetic field, for which a linear partial differential equation (PDE) can be written using a four-dimensional representation of the Lorentz group, the relativistic Dirac equation is the linear PDE

$$\mathrm{i}\sum_{k=0}^{3}\gamma_k\frac{\partial}{\partial x_k}\psi=m\psi,\quad x_0\equiv ct$$

where the γ_k generate the algebra of a representation of the Lorentz group. The operator $\sum(\partial/\partial x_k)\gamma_k$ is a local square root of the relativistically invariant d'Alembert operator $-\partial^2/\partial x_0^2+\Delta-m\cdot 1$.

When one tries to introduce (relativistically invariant) local interactions, one faces the same problem as in the classical mechanics, namely one must introduce relativistically covariant fields (e.g., the electromagnetic field), that is, systems with an infinite number of degrees of freedom. If this field is considered as external, one faces technical problems, which can be overcome in favorable cases. But if one tries to obtain a fully quantized theory (by also quantizing the field) the obstacles become unsurmountable, due also to the nonuniqueness of the representation of the canonical commutation relations if these are taken as the basis of quantization, as in the finite-dimensional case.

In a favorable case (e.g., the interaction of a quantum particle with the quantized electromagnetic field) one can set up a perturbation scheme in a parameter α (the physical value of α in natural units is roughly 1/137). We shall come back later to perturbation schemes in the context of the Schrödinger operator; in the present case one has been able to find procedures (renormalization) by which the series in α that describe relevant physical quantities are well defined term by term. But even in this favorable case, where the sum of the first few terms of the series is in excellent agreement with the experimental data, one has reasons to believe that the series is not convergent, and one does not even know whether the series is asymptotic.

One is led to wonder whether the structure of fields (operator-valued elements in the dual of compactly supported smooth functions on classical spacetime), taken over in a simple way from the field structure of classical electromagnetism, is a valid instrument in the description of phenomena that take place at a scale incomparably smaller than the scale (atomic scale) at which we have reasons to believe that the formalisms of Schrödinger and Heisenberg provide a suitable model for the description of natural phenomena.

The phenomena which are related to the interaction of a quantum nonrelativistic particle interacting with the quantized electromagnetic field take place at the atomic scale. These phenomena have been the subject of very intense research in theoretical physics, mostly within perturbation theory, and the analysis to the first few orders has led to very spectacular results (although there is at present no proof that the perturbation series are at least asymptotic).

In this field rigorous results are scarce, but recently some progress has been made, establishing, among other things, the existence of the ground state (a nontrivial result, because there is no gap separating the ground-state energy from the continuous part of the spectrum) and paving the way for the description of scattering phenomena; the latter result is again nontrivial because the photon field may lead to an anomalous infrared (long-range) behavior, much in the same way that the long-range Coulomb interaction requires a special treatment in nonrelativistic scattering theory.

This contribution to the Encyclopedia is meant to be an introduction to QM and therefore we shall limit ourselves to the basic structure of nonrelativistic theory, which deals with systems of a finite number of particles interacting among themselves and with external (classical) potential fields, leaving for more specialized contributions a discussion of more advanced items in QM and of the successes and failures of a relativistically invariant theory of interaction between quantum particles and quantized fields.

We shall return therefore to basics.

One may begin a section on dynamics in QM by discussing some properties of the solutions of the Schrödinger equation, in particular dispersive effects and the related scattering theory, the problem of bound states and resonances, the case of time-dependent perturbation and the ionization effect, the binding of atoms and molecules, the Rayleigh scattering, the Hall effect and other effects in nanophysics, the various multiscale and adiabatic limits, and in general all the physical problems that

have been successfully solved by Schrödinger's QM (as well as the very many interesting and unsolved problems).

We will consider briefly these issues and the approximation schemes that have been developed in order to derive explicit estimates for quantities of physical interest. Since there are very many excellent reviews of present-day research in QM (e.g., Araki and Ezawa (2004), Blanchard and Dell'Antonio (2004), Cycon *et al.* (1986), Islop and Sigal (1996), Lieb (1990), Le Bris (2005), Simon (2002), and Schlag (2004)) we refer the reader to the more specialized contributions to this Encyclopedia for a detailed analysis and precise statements about the results.

We prefer to come back first to the foundations of the theory; we shall take the point of view of Heisenberg and start discussing the mapping properties of the algebra of observables and of the states. Since transition probabilities play an important role, we consider only transformations α which are such that, for any pair of pure states ϕ_1 and ϕ_2, one has $<\alpha(\phi_1), \alpha(\phi_2)> = <\phi_1, \phi_2>$. We call these maps Wigner automorphisms.

A result of Wigner (see Weyl (1931)) states that if α is a Wigner automorphism then there exists a unique operator U_α, either unitary or antiunitary, such that $\alpha(P) = U_\alpha^* P U_\alpha$ for all projection operators. If there is a one-parameter group of such automorphisms, the corresponding operators are all unitary (but they need not form a group).

A generalization of this result is due to Kadison. Denoting by $I_{1,+}$ the set of density matrices, a Kadison automorphism β is, by definition, such that for all $\sigma_1, \sigma_2 \in I_{1,+}$ and all $0 < s < 1$ one has $\beta(s\sigma_1 + (1-s)\sigma_2) = s\beta(\sigma_1) + (1-s)\beta(\sigma_2)$. For Kadison automorphisms the same result holds as for Wigner's.

A similar result holds for automorphisms of the observables. Notice that the product of two Hermitian operators is not Hermitian in general, but Hermiticity is preserved under Jordan's product defined as $A \times B \equiv (1/2)[AB + BA]$.

A Segal automorphism is, by definition, an automorphism of the Hermitian operators that preserves the Jordan product structure. A theorem of Segal states that γ is a Segal automorphism if and only if there exist an orthogonal projector E, a unitary operator U in $E\mathcal{H}$, and an antiunitary operator V in $(I-E)\mathcal{H}$ such that $\gamma(A) = WAW^*$, where $W \equiv U \oplus V$.

We can study now in more detail the description of the dynamics in terms of automorphism of Wigner or Kadison type when it refers to states and of Segal type when it refers to observables. We require that the evolution be continuous in suitable topologies. The strongest result refers to Wigner's case. One can prove that if a one-parameter group of Wigner automorphism α_t is measurable in the weak topology (i.e., $\alpha_t\sigma(A)$ is measurable in t for every choice of A and σ) then it is possible to choose the $U(t)$ provided by Wigner's theorem in such a way that they form a group which is continuous in the strong topology. Similar results are obtained for the cases of Kadison and Segal automorphism, but in both cases one has to assume continuity of α_t in a stronger topology (the strong operator topology in the Segal case, the norm topology in Kadison's). Weak continuity is sufficient if the operator product is preserved (in this case one speaks of automorphisms of the algebra of bounded operators). The existence of the continuous group $U(t)$ defines a Hamiltonian evolution. One has indeed:

Theorem 1 (Stone). *The map $t \to U(t), t \in R$ is a weakly continuous representation of R in the set of unitary operators in a Hilbert space $\mathcal{H}$ if and only if there exists a self-adjoint operator H on (a dense set of) $\mathcal{H}$ such that $U(t) = e^{itH}$ and therefore*

$$\phi \in D(H) \to i\frac{dU(t)}{dt}\phi = HU(t)\phi \qquad [10]$$

The operator H is called generator of the dynamics described by $U(t)$.

Note In Schrödinger's approach the operator described in Stone's theorem is called Hamiltonian, in analogy with the classical case. In the case of one particle of mass m in R^3 subject to a conservative force with potential energy $V(x)$ it has the following form, in units in which $\hbar = 1$:

$$H = -\frac{1}{2m}\Delta + V(x), \quad \Delta = \sum_k \frac{\partial^2_{x_k}}{\partial x_k^2} \qquad [11]$$

If the potential V depends on time, Stone's theorem is not directly applicable but still the spectral properties of the self-adjoint operators H_t and of the Kernel of the group $\tau \to e^{iH_t\tau}$ are essential to solve the (time-dependent) Schrödinger equation.

The semigroup $t \to e^{-tH_0}$ is usually a positivity-preserving semigroup of contractions and defines a Markov process; in favorable cases, the same is true of $t \to e^{-tH}$ (Feynmann–Kac formula).

There is an analogous situation in the general theory of dynamical systems on a von Neumann algebra; in analogy with the case of elliptic operators, one defines as "dissipation" a map Δ on a von Neumann algebra $\mathcal{M}$ which satisfies $\Delta(a^*a) \geq a^*\Delta(a) + \Delta(a^*)a$ for all $a \in \mathcal{M}$. The positive dissipation Δ is called completely positive if it remains positive after tensorization with $\mathcal{B}(\mathcal{K})$ for any

Hilbert space K. Notice that according to this definition every *-derivation is a completely positive dissipation. For dissipations there is an analog of the theorem of Stinespring, and often bounded dissipation can be written as

$$\Delta(a) = \mathrm{i}[h, a] + \sum V_k^* a V_k - \left(\frac{1}{2}\right) \sum \{V_k^* V_k, a\}$$

for $a \in \mathcal{M}$

(the symbols $\{.,.\}$ denote the anticommutator).

In general terms, by quantization is meant the construction of a theory by deforming a commutative algebra of functions on a classical phase X in such a way that the dynamics of the quantum system can be derived from the prescription of deformation, usually by deforming the Poisson brackets if X is a cotangent bundle $T^*\mathcal{M}$ (Halbut 2002, Landsman 2002). We shall discuss only the Weyl quantization (Weyl 1931) that has its roots in Heisenberg's formulation of QM and refers to the case in which the configuration space is R^N, or, with some variant (Floquet–Zak) the N-dimensional torus. We shall add a few remarks on the Wick (anti-Weyl) quantization. More general formulations are needed when one tries to quantize a classical system defined on the cotangent bundle of a generic variety and even more so if it defined on a generic symplectic manifold.

The Weyl quantization is a mathematically accurate rendering of the essential content of the procedure adopted by Born and Heisenberg to construct dynamics by finding operators which play the role of symplectic coordinates.

Consider a system with one degree of freedom. The first naive attempt would be to find operators $\hat{q}, \hat{p}$ that satisfy the relation

$$[\hat{q}, \hat{p}] \subset \mathrm{i}I \qquad [12]$$

and to construct the Hamiltonian in analogy with the classical case. To play a similar role, the operators $\hat{q}$ and $\hat{p}$ must be self-adjoint and satisfy [12] at least in a weak sense. If both are bounded, [12] implies $\mathrm{e}^{-\mathrm{i}b\hat{p}}\hat{q}\mathrm{e}^{-\mathrm{i}b\hat{p}} = \hat{q} + bI$ (the exponential is defined through a convergent series) and therefore the spectrum of $\hat{q}$ is the entire real line, a contradiction. Therefore, that inclusion sign in [12] is strict and we face domain problems, and as a consequence [12] has many inequivalent solutions ("equivalence" here means "unitary equivalence").

Apart from "pathological" ones, defined on L^2-spaces over multiple coverings of R, there are inequivalent solutions of [12] which are effectively used in QM.

The most common solution is on the Hilbert space $L^2(R)$ (with Lebesgue measure), with $\hat{x}$ defined as the essentially self-adjoint operator that acts on the smooth functions with compact support as multiplication by the coordinate x and $\hat{p}$ is defined similarly in Fourier space. This representation can be trivially generalized to construct operators $\hat{q}_k$ and $\hat{p}_k$ in $L^2(R^N)$.

Another frequently used representation of [12] is on $L^2(S^1)$ (and when generalized to N degrees of freedom, on T^N). In this representation, the operator $\hat{p}$ is defined by $c_k \to kc_k$ on functions $f(\theta) = \sum_{k=-M}^{N} c_k \mathrm{e}^{\mathrm{i}k\theta/2\pi}, 0 \geq M, N < \infty$. In this case the operator $\hat{q}$ is defined as multiplication by the angle coordinate θ. It is easy to check that this representation is inequivalent to the previous one and that [12] is satisfied (as an identity) on the (dense) set of vectors which are in the domain both of $\hat{p}\hat{q}$ and of $\hat{q}\hat{p}$. But notice that the domain of essential self-adjointness of $\hat{p}$ is not left invariant by the action of $\hat{q}$ ($\theta f(\theta)$ is a function on S^1 only if $f(2\pi) = 0$).

We shall denote $\hat{p}$ in this representation by the symbol $\partial/\partial\theta_{\mathrm{per}}$ and refer to it as the Bloch representation. It can be modified by setting the action of $\hat{p}$ as $c_n \to nc_n + \alpha, 0 < \alpha < 2\pi$, and this gives rise to the various Bloch–Zak and magnetic representations.

The Bloch representation can be extended to periodic functions on R^1 noticing that $L^2(R) = L^2(S^1) \otimes l^2(N)$; similarly, the Bloch–Zak and the magnetic representation can be extended to $L^2(R^N)$.

The difference between the representations can be seen more clearly if one considers the one-parameter groups of unitary operators generated by the "canonical operators" $\hat{q}$ and $\hat{p}$. In the Schrödinger representation on $L^2(R)$, these groups satisfy

$$U(a)V(b) = \mathrm{e}^{\mathrm{i}ab} V(b)U(a)$$
$$U(a) = \mathrm{e}^{\mathrm{i}a\hat{q}}, \qquad V(b) = \mathrm{e}^{\mathrm{i}b\hat{p}}$$

and therefore, setting $z = a + \mathrm{i}b$ and $W(z) \equiv \mathrm{e}^{-\mathrm{i}ab/2} V(b)U(a)$ one has

$$W(z)W(z') = \mathrm{e}^{-\mathrm{i}\omega(z,z')/2} W(z + z')$$
$$z \in C, \quad \omega(z, z') = \mathrm{Im}(\bar{z}, z') \qquad [13]$$

The unitary operators $W(z)$ are therefore projective representations of the additive group C. This generalizes immediately to the case of N degrees of freedom; the representation is now of the additive group C^N and ω is the standard symplectic form on C^N.

In the Bloch representation, the unitaries $U(a)V(b)U^*(a)V^*(b)$ are not multiples of the identity, and have no particularly simple form. The map $C^N \ni z \to W(z)$ with the structure [13] is called Weyl system; it plays a major role in QM. The following

theorem has therefore a major importance in the mathematical theory of QM.

Theorem 2 (von Neumann 1965). *There exists only one, modulo unitary equivalence, irreducible representation of the Weil system.*

The proof of this theorem follows a general pattern in the theory of group representations. One introduces an algebra $\mathcal{W}^{(N)}$ of operators

$$W_f \equiv \int f(z)W(z)\mathrm{d}z, \quad f \in L^1(C^N)$$

called Weyl algebra.

It easy to see that $|W_f| = |f|_1$ and that $f \to W_f$ is a linear isomorphism of algebras if one considers $\mathcal{W}^{(N)}$ with its natural product structure and L^1 as a noncommutative algebra with product structure

$$f * g \equiv \int \mathrm{d}z' f(z-z')g(z') \exp \frac{\mathrm{i}}{2}\omega(z,z') \qquad [14]$$

So far the algebra $\mathcal{W}^{(N)}$ is a concrete algebra of bounded operators on $L^2(R^2)$. But it can also be considered an abstract C^*-algebra which we still denote by $\mathcal{W}^{(N)}$.

It is easy to see that, according to [14], if f_0 is chosen to be a suitable Gaussian, then W_{f_0} is a projection operator which commutes with all the W_f's. Moreover, $W_f W_g = \phi_{f,g} W_{f*g}$ for a suitable phase factor ϕ. Considering the Gelfand–Neumark–Segal construction for the C^*-algebra $\mathcal{W}^{(N)}$, one finds that these properties lead to a decomposition of any representation in cyclic irreducible equivalent ones, completing the proof of the theorem.

The Weyl system has a representation (equivalent to the Schrödinger one) in the space $L^2(R^N, g)$, where g is Gauss's measure. This allows an extension in which C^N is replaced by an infinite-dimensional Banach space equipped with a Gauss measure (weak distribution (Segal 1965, Gross 1972, Wiener 1938)). Uniqueness fails in this more general setting (uniqueness is strictly connected with the compactness of the unit ball in C^N). Notice that in the Schrödinger representation (and, therefore, in any other representation) the Hamiltonian for the harmonic oscillator defines a positive self-adjoint operator

$$N = \sum_1^N N_k, \quad N_k = -\frac{\partial^2}{\partial x_{k^2}} + x_k^2 - 1$$

The spectrum of each of the commuting operators N_k consists of the positive integers (including 0) and is therefore called number operator for the kth degree of freedom. The operator N_k can be written as $N_k = a_k^* a_k$, where $a_k = (1/\sqrt{2})(x_k + \partial/\partial x_k)$ and a_k^* is the formal adjoint of a_k in $L^2(R)$. One has $|a_k(N_k+1)^{-1/2}| < 1$. In the domain of N these operators satisfy the following relations (canonical commutation relations)

$$\begin{aligned} [a_k, a_h^*] &= \delta_{k,h}, \qquad [a_h, a_k] = 0 \\ [N_k, a_h] &= -a_h \delta_{h,k}, \qquad [N_h, a_k^*] = a_k^* \delta_{h,k} \end{aligned} \qquad [15]$$

In view of the last two relations, the operator a_k is called the annihilation operator (relative to the kth degree of freedom) and its formal adjoint is called the creation operator. The operators a_k have as spectrum the entire complex plane, the operators a_k^* have empty spectrum; the eigenvectors of N_k are the Hermite polynomials in the variable x_k. The eigenvectors of a_k (i.e., the solutions in $L^2(R)$ of the equation $a_k \phi_\lambda = \lambda \phi_\lambda, \lambda \in C$) are called coherent states; they have a major role in the Bargmann–Fock–Segal quantization and in general in the semiclassical limit.

The operators $\{N_k\}$ generate a maximal abelian system and therefore the space $L^2(R^N)$ has a natural representation as the symmetrized subspace of $\oplus_k (C^N)^k$ (Fock representation). In this representation, a natural basis is given by the common eigenvectors $\phi_{\{n_k\}}, k = 1, \ldots, N$, of the operators N_k. A generic vector can be written as

$$\psi = \sum_{\{n_k\}} c_{\{n_k\}} \phi_{\{n_k\}}, \quad \sum_{\{n_k\}} |c_{\{n_k\}}|^2 < \infty$$

and therefore can be represented by the sequence $c_{\{n_k\}}$.

Notice that the creation operators do not create particles in R^N but rather act as a shift in the basis of the Hermite polynomials.

It is traditional to denote by $\gamma(L^2(R^N))$ the Fock representation (also called second quantization because for each degree of freedom the wave function is written in the quantized basis of the harmonic oscillator) and to denote by $\Gamma(A)$ the lift of a matrix $A \in B(C^N)$. These notations are especially used if C^N is substituted with a Banach space X. This terminology was introduced by Segal in his work on quantization of the wave equation; it is used ever since, mostly in a perturbative context.

In the theory of quantized fields, the space C^N is substituted with a Banach space, X, of functions. In this setting, "second quantization" (Segal 1965, Nelson 1974) considers the state $\phi_{\{n_k\}}$ as representing a configuration of the system in which there are precisely n_k particles in the kth physical state (this presupposes having chosen a basis in the space of distribution on R^3). There is no problem in doing this (Gross 1972) and one can choose for X a suitable Sobolev space (which one depends on the Gaussian measure given in X) if one wants that the

generalization of the commutation relations [15] be of the form $[a^*(f), a(g)] = <f, g>$ with a suitable scalar product $<\cdot, \cdot>$ in X. The problem with quantization of relativistic fields is that, in order to ensure locality, one is forced to use a Sobolev space of negative index (depending on the dimension of physical space), and this gives rise to difficulties in the definition of the dynamics for nonlinear vector fields.

One should notice that in the work of Segal (1965), and then in Constructive field theory (Nelson 1974), the Fock representation is placed in a Schrödinger context exhibiting the relevant operators as acting on a space $L^2(X, g)$, where X is a subspace of the space of Schwartz distributions on the physical space of the particles one wants to describe and g is a suitably defined Gauss measure on X.

The Fock representation is related to the Bargmann–Fock–Segal representation (Bargmann 1967), a representation in a space of holomorhic functions on C^N square integrable with respect to a Gaussian measure. For its development, this representation relies on the properties of Toeplitz operators and on Tauberian estimates. It is much used in the study of the semiclassical limit and in the formulation of QM in systems for which the classical version has, for phase space, a manifold which is not a cotangent bundle (e.g., the 2-sphere).

Remark The Fock representation associated with the Weyl system in the infinite-dimensional context can describe only particles obeying Bose–Einstein statistics; indeed, the states are qualified by their particle content for each element of the basis chosen and there is no possibility of identifying each particle in an N-particle state. This is obvious in the finite-dimensional case: the Hermite polynomial of order 2 cannot be seen as "composed" of two polynomials of order 1.

In the infinite-dimensional context, if one wants to treat particles which obey Fermi–Dirac statistics, one must rely on the Pauli exclusion principle (Pauli 1928), which states that two such particles cannot be in the same configuration; to ensure this, the wave function must be antisymmetric under permutation of the particle symbols. It is a matter of fact (and a theorem in relativistic quantum field theory which follows in that theory from covariance, locality and positivity of the energy (Streater and Wightman 1964) that particles with half-integer spin obey the Fermi–Dirac statistics. Therefore, to quantize such systems, one must introduce (commutation) relations different from those of Weyl. Since it must now be that $(a^*)^2 = 0$, due to antisymmetry, it is reasonable to introduce the following relations (canonical anticommutation relations:

$$\begin{aligned} &\{a_k, a_h^*\} = \delta_{k,h}, \qquad \{a_h, a_k\} = 0 \\ &[N_k, a_h] = -a_h \delta_{h,k}, \quad \{A, B\} \equiv AB - BA \end{aligned} \tag{16}$$

The Hilbert space is now $\otimes^N \mathcal{H}_2$, where $\mathcal{H}_2$ is a two-dimensional complex Hilbert space. Notice that $\mathcal{H}_2$ carries an irreducible two-dimensional representation of $sU(2) \equiv o(3)$ (spin representation) so that this quantization associates spin 1/2 and antisymmetry.

The operators in [16] are all bounded (in fact bounded by 1 in norm). The Fock representation is constructed as in the case of Weyl (see Araki (1988)), with n_k equal 0 or 1 for each index k. The infinite-dimensional case is defined in the same way, and leads to inequivalent irreducible representations (Araki 1988); only in one of them is the number operator defined and bounded below. Some of these representations can be given a Schrödinger-like form, with the introduction of a gauge and an integration formalism based on a trace (Gross 1972). This system is much used in quantum statistical mechanics because it deals with bounded operators and can take advantage of strong results in the theory of C^*-algebras. In the finite-dimensional case (and occasionally also in the general case) it is used in quantum information (the space $\mathcal{H}_2$ is the space of a quantum bit).

Returning to the Weyl system, we now introduce the strictly related Wigner function which plays an important role in the analysis of the semiclassical limit and in the discussion of some scaling limits, in particular the hydrodynamical limit and the Bose–Einstein condensation when $N \to \infty$.

The Wigner function W_ϕ for a pure state ϕ is a real-valued function on the phase space of the classical system which represents the state faithfully. It is defined as

$$W_\psi(x, \xi) = (2\pi)^{-n} \int_{R^n} e^{-i(\xi, x)} \psi\left(x + \frac{y}{2}\right) \bar{\psi}\left(x - \frac{y}{2}\right) dy$$

The Wigner function is not positive in general (the only exceptions are those Gaussian states that satisfy $\Delta(x) \cdot \Delta(p) \geq \hbar$). But is has the interesting property that its marginals reproduce correctly the Born rule. In fact, one has $\int W_\phi(x, \xi)\, dx = |\hat{\phi}(\xi)|^2$. If the function $\phi(t, x)$ $x \in R^n$ is a solution of the free Schrödinger equation $i\hbar \partial\phi/\partial t = -\hbar^2 \Delta$ then its Wigner function satisfies the Liouville (transport) equation $\partial W_\phi/\partial t + \xi \cdot \nabla W = 0$.

The Wigner function is strictly linked with the Weyl quantization. This quantization associates with every function $\sigma(p, x)$ in a given regularity

class an operator $\sigma(D,x)$ (the Weyl symbol of the function σ) defined by

$$(\sigma(D,x)f,g) \equiv \int \sigma(\xi,x)\,W(f,g)(\xi,x)\,\mathrm{d}\xi\,\mathrm{d}x$$

$$W(f,g)(\xi,x) \equiv \int \mathrm{e}^{-\mathrm{i}(\xi,p)} f\left(x+\frac{p}{2}, x-\frac{p}{2}\right)\mathrm{d}p$$

It can be verified that the action of F preserves the Schwartz classes S and S' and is unitary in $L^2(R^{2N})$. Moreover, one has $\sigma(D,x)^* = \bar{\sigma}(D,x)$.

The relation between Weyl's quantization and Wigner functions can be readily seen from the natural duality between bounded operators and pure states:

$$\mathrm{tr}(\hat{A}\,\hat{\rho}) \equiv \int a(p,q)\rho(p,q)\,\mathrm{d}p\,\mathrm{d}q$$

$$\rho(p,q) = \int \mathrm{e}^{\mathrm{i}(p,q')}\rho(q',q)\,\mathrm{d}q'$$

We give now a brief discussion of the general structure of a quantization, and apply it to the Weyl quantization. By quantization of a Hamiltonian system we mean a correspondence, parametrized by a small parameter $\hbar$, between classical observables (real functions on a phase space $\mathcal{F}$) and quantum observables (self-adjoint operators on a Hilbert space $\mathcal{H}$) with the property that the corresponding structures coincide in the limit $\hbar \to 0$ and the difference for $\hbar \neq 0$ can be estimated in a suitable topology.

This last requirement is important for the applications and, from this point of view, Weyl's quantization gives stronger results than the other formalisms of quantization.

We limit our analysis to the case $\mathcal{F} \equiv T^*X$, with $X \equiv R^N$, and we make use of the realization of $\mathcal{H}$ as $L^2(R^N)$.

Let $\{x_i\}$ be Cartesian coordinates in R^N and consider a correspondence $A \to \hat{A}$ that satisfies the following requirements:

1. $A \leftrightarrow \hat{A}$ is linear;
2. $x_k \leftrightarrow \hat{x}_k$ where $\hat{x}_k$ is multiplication by x_k;
3. $p_k \leftrightarrow -\mathrm{i}\hbar\partial/\partial x_k$;
4. if f is a continuous function in R^N, one has $f(x) \leftrightarrow f(\hat{x})$ and $\hat{f}(p) = (Ff)(\hat{x})$, where F denotes a Fourier transform;
5. $L_\zeta \leftrightarrow \hat{L}_\zeta, \zeta \equiv (\alpha,\beta), \alpha,\beta \in R^N$, where L_ζ is the generator of the translations in phase space in the direction ζ and $\hat{L}_\zeta$ is the generator of the one-parameter group $t \to W(t\zeta)$ associated with ζ by the Weyl system.

Note that (1) and (4) imply (2) and (3) through a limit procedure.

Under the correspondence $A \leftrightarrow \hat{A}$, linear symplectic maps correspond to unitary transformations. This is not in general the case for nonlinear maps.

One can prove that conditions (1)–(5) give a complete characterization of the map $A \leftrightarrow \hat{A}$. Moreover, the correspondence cannot be extended to other functions in phase space. Indeed, one has:

Theorem 3 (van Hove). *Let G be the class of functions C^∞ on R^{2N} which are generators of global symplectic flows. For $g \in G$ let $\Phi_g(t)$ be the corresponding group. There cannot exist for every g a correspondence $g \leftrightarrow \hat{g}$, with $\hat{g}$ self-adjoint, such that $\hat{g}(x,p) = g(\hat{x},\hat{p})$.*

We described the Weyl quantization as a correspondence between functions in the Schwartz class S and a class of bounded operators. Weyl's quantization can be extended to a much wider class of functions. Operators that can be so constructed are called Fourier integral operators. One uses the notation $\hat{\sigma} \equiv \sigma(D,x)$.

We have the following useful theorems (Robert 1987):

Theorem 4 *Let $l_1,\ldots,l_K$ be linear functions on R^N such that $\{l_i l_k\} = 0$. Let P be a polynomial and let $\sigma(\xi,x) \equiv P[l_1(\xi,x), l_K(\xi,x)]$. Then*

(i) *$\sigma(D,x)$ maps S in $L^2(R^N)$ and self-adjoint;*
(ii) *if g is continuous, then $(g(\sigma)(D,x) = g(\sigma(D,x))$.*

One proves that $\sigma(D,x)$ extends to a continuous map $S'(X) \to S'(X)$ and, moreover,

Theorem 5 (Calderon–Vaillancourt). *If $\sigma_0 \equiv \sum_{|\alpha|+|\beta|\leq 2N+1} |D_\xi^\alpha D_x^\beta \sigma| < \infty$ the norm of the operator $\sigma(D,x)$ is bounded by σ_0.*

Any operator obtained from a suitable class of functions through Weyl's quantization is called a pseudodifferential operator. If $\sigma(q,p) = P(p)$, where P is a polynomial, $\hat{\sigma}(p,q)$ is a differential operator.

Moreover, if $\sigma(p,x) \in L^2$ then $\sigma(D,x)$ is a Hilbert–Schmidt operator and

$$|\sigma(D,x)|_{\mathrm{HS}} = (2\pi\hbar)^{-n/2}\left[\int |A(z)|^2\,\mathrm{d}z\right]^{1/2}$$

Pseudodifferential operators turn out to be very important in particular in the quantum theory of molecules (Le Bris 2003), where adiabatic analysis and Peierls substitution rules force the use of pseudodifferential operators.

The next important problem in the theory of quantization is related to dynamics.

Let β be a quantization procedure and let $H(p,q)$ be a classical Hamiltonian on phase space. Let A_t be

the evolution of a classical observable A under the flow defined by H and assume that $\beta(A_t)$ is well defined or all t.

Is there a self-adjoint operator $\hat{H}$ such that $\beta(A_t) = e^{it\hat{H}}\beta(A)\,e^{-it\hat{H}}$? If so, can one estimate $|\hat{H} - \beta(H)|$? Conversely, if the generator of the quantized flow is, by definition, $\hat{H}$ (as is usually assumed), is it possible to give an estimate of the difference $|\beta(A_t) - (\beta(A))_t|\phi$ for a dense set of $\phi \in \mathcal{H}$, where $A_t \equiv e^{it\hat{H}}Ae^{-it\hat{H}}$, or to estimate $|\tilde{A}_t - A_t|_\infty$, where $\tilde{A}_t$ is defined by $\beta(\tilde{A}_t) = (\beta(A))_t$. Is it possible to write an asymptotic series in $\hbar$ for the differences?

For the Weyl quantization some quantitative results have been obtained if one makes use of the semiclassical observables (Robert 1987). We shall not elaborate further on this point.

For completeness, we briefly mention another quantization procedure which is often used in mathematical physics.

Wick Quantization

This quantization assigns positive operators to positive functions, but does not preserve polynomial relations. It is strictly related to the Bargmann–Fock–Segal representation.

Call coherent state centered in the point (y, η) of phase space the normalized solution of $(i\hat{p} + \hat{x} - i\eta + x)\phi_{y,\eta}(x) = 0$.

Wick's quantization of the classical observable A is by definition the map $A \to \mathrm{Op}^{\mathrm{W}}(A)$, where

$$\mathrm{Op}^{\mathrm{W}}(A)\psi \equiv (2\pi\hbar)^{-n}\int A(y,\eta)(\psi, \bar{\phi}_{y,\eta})\phi_{y,\eta}\,dy\,d\eta$$

One can prove, either directly or going through Weyl's representation, that

1. if $A \geq 0$ then $\mathrm{Op}_\hbar^{\mathrm{W}}(A) \geq 0$;
2. the Weyl symbol of the operator $\mathrm{Op}_\hbar^{\mathrm{W}}(A)$ is
$$(\pi\hbar)^{-n}\int\int A(y,\eta)e^{-\frac{i}{\hbar}[(x-y)^2+(\xi-\eta)^2]}\,dy\,d\eta$$
3. for every $A \in O(0)$ one has $\|\mathrm{Op}_\hbar^{\mathrm{W}}(A) - \hat{A}\| = O(\hbar)$.

Wick's quantization associates with every vector $\phi \in \mathcal{H}$ a positive Radon measure μ_ϕ in phase space, called Husimi measure. It is defined by $\int A\,d\mu_\psi = (\mathrm{Op}_\hbar^{\mathrm{W}}(A)\psi \cdot \psi)$, $A \in S(z)$. Wick's quantization is less adapted to the treatment of nonrelativistic particles, in particular Eherenfest's rule does not apply, and the semiclassical propagation theorem has a more complicated formulation. It is very much used for the analysis in Fock space in the theory of quantized relativistic fields, where a special role is assigned to Wick ordering, according to which the polynomials in $\hat{x}_\hbar$ and $\hat{p}_\hbar$ are reordered in terms of creation and annihilation operators by placing all creation operators to the left.

We now come back to Schrödinger's equation and notice that it can be derived within Heisenberg's formalism and Weyl's quantization scheme from the Hamiltonian of an N-particle system in Hamiltonian mechanics (at least if one neglects spin, which has no classical analog).

Apart from (often) inessential parameters, the Schrödinger equation for N scalar particles in R^3 can be written as

$$i\hbar\frac{\partial\phi}{\partial t} = \sum_{k=1}^{N}(i\hbar\nabla_k + A_k)^2\phi + V\phi \equiv H\phi \qquad [17]$$
$$\phi \in L^2(R^{3N})$$

where A_k are vector-valued functions (vector potentials) and $V = V_k(x_k) + V_{i,k}(x_i - x_k)$ are scalar-valued function (scalar potentials) on R^3.

Typical problems in Schrödinger's quantum mechanics are:

1. Self-adjointness of H, existence of bound states (discrete spectrum of the operator), their number and distribution, and, in general, the properties of the spectrum.
2. Existence, completeness, and continuity properties of the wave operators
$$W_\pm \equiv s - \lim_{\mp\infty} e^{itH_0}\,e^{-itH} \qquad [18]$$
and the ensuing existence and properties of the S-matrix and of the scattering cross sections. In [18] H_0 is a suitable reference operator, usually $-\Delta$ (with periodic boundary conditions if the potentials are periodic in space), for which Schrödinger's equation can be somewhat analytically controlled.
3. Existence and property of a semiclassical limit.

In [17] and [18] we have implicitly assumed that H is time independent; very interesting problems arise when H depends on time, in particular if it is periodic or quasiperiodic in time, giving rise to ionization phenomena. In the periodic case, one is helped by Floquet's theory, but even in this case many interesting problems are still unsolved.

If the potentials are sufficiently regular, the spectrum of H consists of an absolutely continuous part (made up of several bands in the space-periodic case) and a discrete part, with few accumulation points.

On the contrary, if $V(x, \omega)$ is a measurable function on some probability space Ω, with a suitable distribution (e.g., Gaussian), the spectrum may have totally different properties almost surely.

For example, in the case $N = 1$ (so that the terms $V_{i,j}$ are absent) in one and two spatial dimensions the spectrum is pure point and dense, with eigenfunctions which decrease at infinity exponentially fast (although not uniformly); as a consequence, the evolution group does not give rise to a dispersive motion. The same is true in three dimensions if the potential is sufficiently strong and the kinetic energy content of the initial state is sufficiently limited. This very interesting behavior is due roughly to the randomness of the "barriers" generated by the potential and is also present, to a large extent, for potentials quasiperiodic in space (Pastur and Figotin 1992).

In these as well as in most problems related to Schrödinger's equation, a crucial role is taken by the resolvent operator $(H - \lambda I)^{-1}$, where λ is any complex number outside the spectrum of H; many of the results are obtained when the difference $(H - \lambda I)^{-1} - (H_0 - \lambda I)^{-1}$ is a compact operator.

Problems of type (1) and (2) are of great physical interest, and are of course common with theoretical physics and quantum chemistry (Le Bris 2003), although the instruments of investigation are somewhat different in mathematical physics. The semiclassical limit is often more of theoretical interest, but its analysis has relevance in quantum chemistry and its methods are very useful whenever it is convenient to use multiscale methods, as in the study of molecular spectra.

We start with a brief description of point (3); it provides a valid instrument in the description of quantum-mechanical systems at a scale where it is convenient to use units in which the physical constant $\hbar$ has a very small value ($\hbar \simeq 10^{-27}$ in CGS units). From Heisenberg's commutation relations, $[\hat{x}, \hat{p}] \subset \hbar I$, it follows that the product of the dispersion (uncertainty) of the position and momentum variables is proportional to $\hbar$ and therefore at least one of these two quantities must have very large values (compared to $\hbar$). One considers usually the case in which these dispersions have comparable values, which is therefore very small, of the order of magnitude $\hbar^{1/2}$ (but very large as compared with $\hbar$). In order to make connection with the Hamilton–Jacobi formalism of classical mechanics one can also consider the case in which the dispersion in momentum is of the order $\hbar$ (the WKB method).

The semiclassical limit takes advantage mathematically from the fact that the parameter $\hbar$ is very small in natural units, and performs an asymptotic analysis, in which the terms of "lowest order" are exactly described and the difference is estimated. The problem one faces is that the Schrödinger equation becomes, in the "mathematical limit" $\hbar \to 0$, a very singular PDE (the coefficients of the differential terms go to zero in this limit).

Dividing each term of the equation by $\hbar$ (because we do not want to change the scale of time) leads, in the case of one quantum particle in R^3 in potential field $V(x)$ (we treat, for simplicity, only this case), to the equation

$$\mathrm{i}\frac{\partial \phi(x,t)}{\partial t} = -\hbar \Delta \phi(x,t) + \hbar^{-1} V(x)\phi(x,t) \qquad [19]$$

It is convenient therefore to "rescale" the spatial variables by a factor $\hbar^{1/2}$ (i.e., choose different units) setting $x = \sqrt{\hbar}X$ and look for solutions of [19] which remain regular in the limit $\hbar \to 0$ as functions of the rescaled variable X. One searches therefore for solutions that on the "physical scale" have support that becomes "vanishingly small" in the limit. It is therefore not surprising that, in the limit, these solutions may describe point particles; the main result of semiclassical analysis is that he coordinates of these particles obey Hamilton's laws of classical mechanics.

This can be roughly seen as follows (accurate estimates are needed to make this empirical analysis precise). Using multiscale analysis, one may write the solution in the form $\phi(X, x, t)$ and seek solutions which are smooth in X and x. Both terms on the right-hand side of [19] contain contributions of order -2 and -1 in $\sqrt{\hbar}$ and in order to have regular solutions one must have cancellations between equally singular contributions. For this, one must perform an expansion to the second order of the potential (assumed at least twice differentiable) around a suitable trajectory $q(t)$, $q \in R^3$, and choose this trajectory in such a way that the cancellations take place.

A formal analysis shows that this is achieved only if the trajectory chosen is precisely a solution of the classical Lagrange equations. Of course, a more refined analysis and good estimates are needed to make this argument precise, and to estimate the error that is made when one neglects in the resulting equation terms of order $\sqrt{\hbar}$; in favorable cases, for each chosen T the error in the solution for most initial conditions of the type described is of order $\sqrt{\hbar}$ for $|t| < T$.

This semiclassical result is most easily visualized using the formalism of Wigner functions (the technical details, needed to to make into a proof the formal arguments, take advantage of regularity estimates in the theory of functions).

In natural units, one defines

$$W_{\hbar,\rho}(x,\xi,t) = \left(\frac{\mathrm{i}}{2\pi}\right)^N W_\rho\left(x, \frac{\xi}{\hbar}, t\right)$$

In terms of the Wigner function $W_{\hbar,\rho}$ the Schrödinger equation [19] takes the form

$$\frac{\partial f^\hbar}{\partial t} + \xi \cdot \nabla_x f^\hbar + K_\hbar * f^\hbar = 0 \qquad [20]$$
$$\rho^\hbar(t=0) = \rho_0(\hbar)$$

where

$$K_\hbar = \frac{\mathrm{i}}{(2\pi)^N} \mathrm{e}^{-\mathrm{i}\xi,y\hbar^{-1}} \left[V\left(x + \frac{\hbar y}{2}\right) - V\left(x - \frac{\hbar y}{2}\right) \right]$$

It can be proved (Robert 1987) that if the potential is sufficiently regular and if the initial datum converges in a suitable topology to a positive measure f_0, then, for all times, $W_{\hbar,\rho}(x,t)$ converges to a (weak) solution of the Liouville equation

$$\frac{\partial f}{\partial t} + \xi \cdot \nabla_x f - \nabla V(x) \cdot \nabla_\xi f = 0$$

This leads to the semiclassical limit if, for example, one considers a sequence of initial data ρ_{ϕ_n} where ϕ_n is a sequence of functions centered at x_0 with Fourier transform centered at p_0 and dispersion of order $\hbar^{1/2}$ both in position and in momentum. In this case, the limit measure is a Dirac measure centered on the classical paths.

In the course of the proof of the semiclassical limit theorem, one becomes aware of the special status of the Hamiltonians that are at most quadratic in $\hat{x}$ and $\hat{p}$. Indeed, it is easy to verify that for these Hamiltonians the expectation values of $\hat{x}$ and $\hat{p}$ obey the classical equation of motion (P Ehrenfest rule).

From the point of view of Heisenberg, this can be understood as a consequence of the fact that operators at most bilinear in a and a^* form an algebra $\mathcal{D}$ under commutation and, moreover, the homogeneous part of order 2 is a closed subalgebra such that its action on $\mathcal{D}$ (by commutation) has the same structure as the algebra of generators of the Hamiltonian flow and its tangent flow. Apart from (important) technicalities, the proof of the semiclassical limit theorem reduces to the proof that one can estimate the contribution of the terms of order higher than 2 in the expansion of the quantum Hamiltonian at the classical trajectory as being of order $\hbar^{1/2}$ in a suitable topology (Hepp 1974).

We end this overview by giving a brief analysis of problems (1) and (2), which refer to the description of phenomena that are directly accessible to comparison with experimental data, and therefore have been extensively studied in theoretical physics and quantum chemistry (Mc Weeny 1992); some of them have been analyzed with the instruments of mathematical physics, often with considerable success. We give here a very naive introduction to these problems and refer the reader to the more specialized contributions to this Encyclopedia for a rigorous analysis and exact statements.

Of course, most of the problems of physical interest are not "exactly solvable," in the sense that rarely the final result is given explicitly in terms of simple functions. As a consequence, exact numerical results, to be compared with experimental data, are rarely obtained in physically relevant problems, and most often one has to rely on approximation schemes with (in favorable cases) precise estimates on the error.

Formal perturbation theory is the easiest of such schemes, but it seldom gives reliable results to physically interesting problems. One writes

$$H_\epsilon \equiv H + \epsilon V \qquad [21]$$

where ϵ is a small real parameter, and sets a formal scheme in case (1) by writing

$$H_\epsilon \phi_\epsilon \equiv E_\epsilon \phi_\epsilon, \quad E_\epsilon \equiv \sum_0^\infty \epsilon^k E_k, \quad \phi_\epsilon \equiv \sum_0^\infty \epsilon^k \phi_k$$

and, in case (2), iterating Duhamel's formula

$$\mathrm{e}^{-\mathrm{i}tH_\epsilon} = \mathrm{e}^{-\mathrm{i}tH_0} + \mathrm{i}\epsilon \int_0^t \mathrm{e}^{-\mathrm{i}(t-s)H_\epsilon} V \mathrm{e}^{-\mathrm{i}sH_0} \mathrm{d}s \qquad [22]$$

Very seldom the perturbation series converges, and one has to resort to more refined procedures.

In some cases, it turns out to be convenient to consider the formal primitive $\tilde{E}_\epsilon$ of E_ϵ (as a differentiable function of ϵ) and prove that it is differentiable in ϵ for $0 < \epsilon < \epsilon_0$ (but not for $\epsilon = 0$). In favorable cases, this procedure may lead to

$$E_\epsilon = \sum_0^N \epsilon^k E_k + R_N(\epsilon), \quad \lim_{N\to\infty} |R_N|(\epsilon) = +\infty$$

with explicit estimates of $|R_N(\epsilon)|$ for $0 \le \epsilon < \epsilon_0$.

Re-summation techniques of the formal power series may be of help in some cases.

The estimate of the lowest eigenvalues of an operator bounded below is often done by variational analysis, making use of min–max techniques applied to the quadratic form $Q(\phi) \equiv (\phi, H\phi)$.

Semiclassical analysis can be useful to search for the distribution of eigenvalues and in the study of the dynamics of states whose dispersions both in position and in momentum are very large in units in which $\hbar = 1$.

A case of particular interest in molecular and atomic physics occurs when the physical parameters which appear in H_ϵ (typically the masses of the particles involved in the process) are such that one

can *a priori* guess the presence of coordinates which have a rapid dependence on time (fast variables) and a complementary set of coordinates whose dependence on time is slow. This suggests that one can try an asymptotic analysis, often in connection with adiabatic techniques. Seldom one deals with cases in which the hypotheses of elementary adiabatic theorems are satisfied, and one has to refine the analysis, mostly through subtle estimates which ensure the existence of quasi invariant subspaces.

Asymptotic techniques and refined estimates are also needed to study the effective description of a system of N interacting identical particles when N becomes very large; for example, in statistical mechanics, one searches for results which are valid when $N \to \infty$.

The most spectacular results in this direction are the proof of stability of matter by E Lieb and collaborators, and the study of the phenomenon of Bose–Einstein condensation and the related Gross–Pitaevskii (nonlinear Schrödinger) equation. The experimental discovery of the state of matter corresponding to a Bose–Einstein condensate is a clear evidence of the nonclassical behavior of matter even at a comparatively macroscopic size. From the point of view of mathematical physics, the ongoing research in this direction is very challenging.

One should also recognize the increasing role that research in QM is taking in applications, also in connection with the increasing success of nanotechnology. In this respect, from the point of view of mathematical physics, the study of nanostructure (quantum-mechanical systems constrained to very small regions of space or to lower-dimensional manifolds, such as sheets or graphs) is still in its infancy and will require refined mathematical techniques and most likely entirely new ideas.

Finally, one should stress the important role played by numerical analysis (Le Bris 2003) and especially computer simulations. In problems involving very many particles, present-day analytical techniques provide at most qualitative estimates and in favorable cases bounds on the value of the quantities of interest. Approximation schemes are not always applicable and often are not reliable.

Hints for a progress in the mathematical treatment of some relevant physical phenomena of interest in QM (mostly in condensed matter physics) may come from the *ab initio* analysis made by simulations on large computers; this may provide a qualitative and, to a certain extent, quantitative behavior of the solutions of Schrödinger's equation corresponding to "typical" initial conditions. In recent times the availability of more efficient computing tools has made computer simulation more reliable and more apt to concur with mathematical investigation to a fuller comprehension of QM.

Interpretation Problems

In this section we describe some of the conceptual problems that plague present-day QM and some of the attempts that have been made to cure these problems, either within its formalism or with an altogether different approach.

Approaches within the QM Formalism

We begin with the approaches "from within." We have pointed out that the main obstacle in the measurement problem is the description of what occurs during an act of measurement. Axiom III claims that it must be seen as a "destruction" act, and the outcome is to some extent random. The final state of the system is one of the eigenstates of the observable, and the dependence on the initial state is only through an *a priori* probability assignment; the act of measurement is therefore not a causal one, contrary to the (continuous) causal reversible description of the interaction with the environment. One should be able to distinguish *a priori* the acts of measurement from a generic interaction.

There is a further difficulty. Due to the superposition principle, if a system $\mathcal{S}$ on which we want to make a measurement of the property associated with the operator A "interacts" with an instrument $\mathcal{I}$ described by the operator S, the final state ξ of the combined system will be a coherent superposition of tensor product of (normalized) eigenstates of the two systems

$$\xi = \sum_{n,m} c_{n,m} \phi_n^A \otimes \psi_m^S, \quad \sum_{n,m} |c_{n,m}|^2 = 1 \qquad [23]$$

Measurement as described by Axiom III of QM claims that once the measurement is over, the measured system is, with probability $\sum_m |c_{n,m}|^2$, in the state ϕ_n^A and the instrument is in a state which carries the information about the final state of the system (after all, what one reads at the end is an indicator of the final state of the instrument).

It is therefore convenient to write ξ in the form

$$\xi = \sum d_n \phi_n^A \otimes \zeta_n, \quad \sum_n |d_n|^2 = 1 \qquad [24]$$

(this defines ζ_n if the spectrum of A is pure point and nondegenerate). It is seen from [24] that, due to the reduction postulate, we know that the the measured system is in the state $\phi_{n_0}^A$ if a measurement of an observable T with nondegenerate spectrum,

eigenvectors $\{\zeta_n\}$, and eigenvalues $\{z_n\}$ gives the results z_{n_0}.

Along these lines, one does not solve the measurement problem (the outcome is still probabilistic) but at least one can find the reason why the measuring apparatus may be considered "classical."

It is more convenient to go back to [23] and to assume that one is able to construct the measuring apparatus in such a way that one divides (roughly) its pure (microscopic) states in sets Φ_n (each corresponding to a "macroscopic" state) which are (roughly) in one-to-one correspondence to the eigenstates of A. The sets Φ_n contain a very large number, N_{Φ_n}, of elements, so that the sets Φ_n need not be given with extreme precision. And the sets Φ_n must be in a sense "stable" under small external perturbations.

It is clear from this rough description that the apparatus should contain a large number of small components and still its interaction with the "small" system A should lead to a more or less sudden change of the sets Φ_n.

A concrete model of this mechanism has been proposed by K Hepp (1972) for the case when A is a 2×2 matrix, and the measuring apparatus is made of a chain of N spins, $N \to \infty$; the analysis was recently completed by Sewell (2005) with an estimate on the error which is made if N is finite but large. This is a dynamical model, in which the observable A (a spin) interacts with a chain of spins ("moves over the spins") leaving the trace of its passage. It is this trace (final macroscopic state of the apparatus) which is measured and associated with the final state of A. The interaction is not "instantaneous" but may require a very short time, depending on the parameters used to describe the apparatus and the interaction.

We call "decoherence" the weakening of the superposition principle due to the interaction with the environment.

Two different models of decoherence have been analyzed in some detail; we shall denote them thermal-bath model and scattering model; both are dynamical models and both point to a solution, to various extents, of the problem of the reduction to a final density matrix which commutes with the operator A (and therefore to the suppression of the interference terms).

The thermal-bath model makes use of the Heisenberg representation and relies on results of the theory of C^*-algebras. This approach is closely linked with (quantum) statistical mechanics; its aim is to prove, after conditioning with respect to the degrees of freedom of the bath, that a special role emerges for a commuting set of operators of the measured system, and these are the observables that specify the outcome of the measurement in probabilistic terms.

The scattering approach relies on the Schrödinger approach to QM, and on results from the theory of scattering. This approach describes the interaction of the system S (typically a heavy particle) with an environment made of a large number of light particles and seeks to describe the state of S after the interaction when one does not have any information on the final state of the light particle. One seeks to prove that the reduced density matrix is (almost) diagonal in a given representation (typically the one given by the spatial coordinates). This defines the observable (typically, position) that can be measured and the probability of each outcome.

Both approaches rely on the loss of information in the process to cancel the effect of the superposition principle and to bring the measurement problem within the realm of classical probability theory. None of them provides a causal dependence of the result of the measurement on the initial state of the system.

We describe only very briefly these attempts.

In its more basic form, the "scattering approach" has as starting point the Schrödinger equation for a system of two particles, one of which has mass very much smaller than the other one. The heavy particle may be seen as representing the system on which a measurement is being made. The outline of the method of analysis (which in favorable cases can be made rigorous) (Joos and Zeh 1985, Tegmark 1993) is the following. One chooses units in which the mass of the heavy particle is 1, and one denotes by ϵ the mass of the light particle. If x is the coordinate of the heavy particle and y that of the light one, and if the initial state of the system is denoted by $\Phi_0(x, y)$, the solution of the equation for the system is (apart from inessential factors)

$$\Phi_t = \exp\{i(-\Delta_x - \epsilon^{-1}\Delta_y + W(x) + V(x-y))t\}\Phi_0$$

Making use of center-of-mass and relative coordinates, one sees that when ϵ is very small one should be able to describe the system on two timescales, one fast (for the light particle) and one slow (for the heavy one) and, therefore, place oneself in a setting which may allow the use of adiabatic techniques. In this setting, for the measure of the heavy particle (e.g., its position) one may be allowed to consider the light particle in a scattering regime, and use the wave operator corresponding to a potential $V_x(y) \equiv V(y-x)$.

Taking the partial trace with respect to the degrees of freedom of the light particle (this

corresponds to no information of its final state) one finds, at least heuristically, that the state of the heavy particle is now described (due to the trace operation) by a density matrix σ for which in the coordinate representation the off-diagonal terms $\sigma_{x,x'}$ are slightly suppressed by a factor $\xi_{x,x'} = 1 - (W_x^+\psi, W_{x'}^+\psi)$ where ψ represents the initial state of the light particle and W_x^+ is the wave operator for the motion of the light particle in the potential ϵV_x. One must assume that function ϕ which represents the initial state of the heavy particle is sufficiently localized so that $\xi_{x,x'} < 1$ for every $x' \neq x$ in its support.

If the environment is made of very many particles (their number $N(\epsilon)$ must be such that $\lim_{\epsilon \to 0} \epsilon N(\epsilon) = \infty$) and the heavy particle can be supposed to have separate interactions with all of them, the off-diagonal elements of the density matrix tend to 0 as $\epsilon \to 0$ and the resulting density matrix tends to have the form $\Phi(x, x') = \delta(x - x')$ $\rho(x), \rho(x) \geq 0$, $\int \rho(x)\, dx = 1$. If it can be supposed that all interactions take place within a time $T(\epsilon) \leq \epsilon^\alpha$, $\alpha > 0$ one has $\rho(x) = |\psi(x)|^2$.

If the interactions are not independent, the analysis becomes much more involved since it has to be treated by many-body scattering theory; this suggests that the scattering approach can be hardly used in the context of the "thermal-bath model." In any case, the selection of a "preferred basis" (the coordinate representation) depends on the fact that one is dealing with a scattering phenomenon. A few steps have been made for a rigorous analysis (Teta 2004) but we are very far from a mathematically satisfactory answer.

The thermal-bath approach has been studied within the algebraic formulation of QM and stands on good mathematical ground (Alicki 2002, Blanchard *et al.* 2003, Sewell 2005). Its drawback is that it is difficult to associate the formal scheme with actual physical situations and it is difficult to give a realistic estimate on the decoherence time.

The thermal-bath approach attributes the decoherence effect to the practical impossibility of distinguishing between a vast majority of the pure states of the systems and the corresponding statistical mixtures. In this approach, the observables are represented by self-adjoint elements of a weakly closed subalgebra $\mathcal{M}$ of all bounded operators $\mathcal{B}(\mathcal{H})$ on a Hilbert space $\mathcal{H}$. This subalgebra may depend on the measuring apparatus (i.e, not all the apparatuses are fit to measure a set of observables). A "classical" observable by definition commutes with all other observables and therefore must belong to the center of $\mathcal{A}$ which is isomorphic to a collection of functions on a probability space $\mathcal{M}$. So the appearance of classical properties of a quantum system corresponds to the "emergence" of an algebra with nontrivial center. Since automorphic evolutions of an algebra preserve its center, this program can be achieved only if we admit the loss of quantum coherence, and this requires that the quantum systems we describe are open and interact with the environment, and moreover that the commutative algebra which emerges be stable for time evolution.

It may be shown that one must consider quantum environment in the thermodynamic limit, that is, consider the interaction of the system to be measured with a thermal bath. A discussion of the possible emergence of classical observables and of the corresponding dynamics is given by Gell-Mann (1993). In all these approaches, the commutative subalgebra is selected by the specific form of the interaction; therefore, the measuring apparatus determines the algebra of classical observables.

On the experimental side, a number of very interesting results have been obtained, using very refined techniques; these experiments usually also determine the "decoherence time." The experimental results, both for the collision model (Hornberger *et al.* 2003) and for the thermal-bath model (Hackermueller *et al.* 2004), are done mostly with fullerene (a molecule which is heavy enough and is not deflected too much after a collision with a particle of the gas). They show a reasonable accordance with the (rough) theoretical conclusions.

The most refined experiments about decoherence are those connected with quantum optics (circularly polarized atoms in superconducting cavities). These are not related to the wave nature of the particles but in a sense to the "wave nature" of a photon as a single unit. The electromagnetic field is now regarded as an incoherent superposition of states with an arbitrarily large number of photons. Polarized photons can be produced one by one, and they retain their individuality and their polarization until each of them interacts with "the environment" (e.g., the boundary of the cavity or a particle of the gas). In a sense, these experimental results refer to a "decoherence by collision" theory.

The experiments by Haroche (2003) prove that coherence may persist for a measurable interval of time and are the most controlled experiments on coherence so far.

Other Approaches

We end this section with a brief discussion of the problem of "hidden variables" and a presentation of an entirely different approach to QM, originated by

D Bohm (1952) and put recently on firm mathematical grounds by Duerr *et al.* (1999). The approach is radically different from the traditional one and it is not clear at present whether it can give a solution to the measurement problem and a description of all the phenomena which traditional QM accounts for. But it is very interesting from the point of view of the mathematics involved.

We have remarked that the formulation of QM that is summarized in the three axioms given earlier has many unsatisfactory aspects, mainly connected with the superposition principle (described in its extremal form by the Schrödinger's cat "paradox") and with the problem of measurement which reveals, for example, through the Einstein–Rosen–Podolski "paradox," an intrinsic nonlocality if one maintains that their "objective" properties can be attributed to systems which are far apart. From the very beginning of QM, attempts have been made to attribute these features to the presence of "hidden variables"; the statistical nature of the predictions of QM is, from this point of view, due to the incompleteness of the parameters used to describe the systems. The impossibility of matching the statistical prediction of QM (confirmed by experimental findings) with a local theory based on hidden variables and classical probability theory has been known for sometime (Kochen and Specker 1967), also through the use of "Bell inequalities" (Bell 1964) among correlations of outcomes of separate measurements performed on entangled system (mainly two photons or two spin-1/2 particles created in a suitable entangled state).

A proof of the intrinsic nonlocality of QM (in the above sense) was given by L Hardy (see Haroche (2003)).

While experimental results prove that one cannot substitute QM with a "naive" theory of hidden variables, more refined attempts may have success. We shall only discuss the approach of Bohm (following a previous attempt by de Broglie) as presented in Duerr *et al.* (1999). It is a dynamical theory in which representative points follow "classical paths" and their motion is governed by a time-dependent vector "velocity" field (in this sense, it is not Newtonian). In a sense, Bohmian mechanics is a minimal completion of QM if one wants to keep the position as primitive observable. To these primitive objects, Bohm's theory adds a complex-valued function ϕ (the "guiding wave" in Bohm's terminology) defined on the configuration space $\mathcal{Q}$ of the particles. In the case of particles with spin, the function ϕ is spinor-valued. Dynamics is given by two equations: one for the coordinates of the particles and one for the guiding wave. If $x \equiv x_1, \ldots, x_N$ describes the configuration of the points, the dynamics in a potential field $V(x)$ is described in the following way: for the wave ϕ by a nonrelativistic Schrödinger equation with potential V and for the coordinates by the ordinary differential equation (ODE)

$$\dot{x}_k = (\hbar/m_k)\mathrm{Im}\left[\frac{\phi^* \nabla_k \phi}{\phi^* \phi}\right](x), \quad x_k \in R^3$$

where m_k is the mass of the mth particle.

Notice that the vector field is singular at the zeros of the wave function, therefore global existence and uniqueness must be proved. To see why Bohmian mechanics is empirically equivalent to QM, at least for measurement of position, notice that the equation for the points coincides with the continuity equation in QM. It follows that if one has at time zero a collection of points distributed with density $|\phi_0|^2$, the density at time t will be $|\phi(t)|^2$ where $\phi(t)$ is the solution of the Schrödinger equation with initial datum ϕ_0.

Bohm (1952) formulated the theory as a modification of Newton's laws (and in this form it has been widely used) through the introduction of a "quantum potential" V_Q. This was achieved by writing the wave function in its polar form $\phi = Re^{iS/\hbar}$ and writing the continuity equation as a modified Hamilton–Jacobi equation. The version of Bohm's theory discussed in Duerr *et al.* (1999) introduces only the guiding wave function and the coordinates of the points, and puts the theory on firm mathematical grounds. Through an impressive series of mathematical results, these authors and their collaborators deal with the completeness of the velocity vector field, the asymptotic behavior of the points trajectories (both for the scattering regime and for the trapped trajectories, which are shown to correspond to bound states in QM), with a rigorous analysis of the theorem on the flux across a surface (a cornerstone in scattering theory) and the detailed analysis of the "two-slit" experiment through a study of the interaction with the measuring apparatus. The theory is completely causal, both for the trajectories of the points and for the time development of the pilot wave, and can also accommodate points with spin. It leads to a mathematically precise formulation of the semiclassical limit, and it may also resolve the measurement problem by relating the pilot wave of the entire system to its approximate decomposition in incoherent superposition of pilot wave associated with the particle and to the measuring apparatus (this would be the way to see the "collapse of the wave function" in QM). A weak point of this approach is the relation of the representative points with observable quantities.

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Introductory Article: Topology

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Introduction

This will be an elementary introduction to general topology. We shall not even touch upon algebraic topology, which will be dealt with in Cohomology Theories, although in some mathematics departments it is introduced in an advanced undergraduate course.

We believe such an elementary article is useful for the encyclopaedia, purely for quick reference. Most of the concepts will be familiar to physicists, but usually in a general rather vague sense. This article will provide the rigorous definitions and results whenever they are needed when consulting other articles in the work. To make sure that this is the case, we have in fact experimentally tested the article on physicists for usefulness.

Topology is very often described as "rubber-sheet geometry," that is, one is allowed to deform objects without actually breaking them. This is the all-important concept of continuity, which underlies most of what we shall study here.

We shall give full definitions, state theorems rigorously, but shall not give any detailed proofs. On the other hand, we shall cite many examples, with a view to applications to mathematical physics, taking for granted that familiar more advanced concepts there need not be defined. By the same token, the choice of topics will also be so dictated.

Essential Concepts

Definition 1 Let X be a set. A collection $\mathcal{T}$ of subsets of X is called a *topology* if the following are satisfied:

(i) $\emptyset, X \in \mathcal{T}$.

(ii) Let $\mathcal{I}$ be an index set. then

$$A_\alpha \in \mathcal{T}, \alpha \in \mathcal{I} \Longrightarrow \bigcup_{\alpha \in \mathcal{I}} A_\alpha \in \mathcal{T}$$

(iii) $A_i \in \mathcal{T}, i = 1, \ldots, n \Longrightarrow \bigcap_{i=1}^{n} A_i \in \mathcal{T}$.

Definition 2 A member of the topology $\mathcal{T}$ is called an *open set* (of X with topology $\mathcal{T}$).

Remark The last two properties are more easily put as *arbitrary* unions of open sets are open, and *finite* intersections of open sets are open. One can easily see the significance of this: if we take the "usual topology" (which will be defined in due course) of the real line, then the intersection of all open intervals $(-1/n, 1/n), n$ a positive integer, is just the single point $\{0\}$, which is manifestly not open in the usual sense.

Example If we postulate that $\emptyset$, and the entire set X, are the only open subsets, we get what is called the *indiscrete* or *coarsest* topology. At the other extreme, if we postulate that all subsets are open, then we get the *discrete* or *finest* topology. Both seem quite unnatural if we think in terms of the real line or plane, but in fact it would be more unnatural to explicitly exclude them from the definition. They prove to be quite useful in certain respects.

Definition 3 A subset of X is *closed* if its complement in X is open.

Remarks

(i) One could easily build a topology using closed sets instead of open sets, because of the simple relation that the complement of a union is the intersection of the complements.

(ii) From the definitions, there is nothing to prevent a set being both open and closed, or neither open nor closed. It is a common mistake to suppose otherwise.

Definition 4 A set equipped with a topology is called a *topological space* (with respect to the given topology). Elements of a topological space are sometimes called *points*.

Definition 5 Let $x \in X$. A *neighborhood* of x is a subset of X containing an open set which contains x.

Remark This seems a clumsy definition, but turns out to be more useful in the general case than restricting to open neighborhoods, which is often done.

Definition 6 A subcollection of open sets $\mathcal{B} \subseteq \mathcal{T}$ is called a *basis* for the topology $\mathcal{T}$ if every open set is a union of sets of $\mathcal{B}$.

Definition 7 A subcollection of open sets $\mathcal{S} \subseteq \mathcal{T}$ is called a *sub-basis* for the topology $\mathcal{T}$ if every open set is a union of finite intersections of sets of $\mathcal{S}$.

Definition 8 The *closure* $\bar{A}$ of a subset A of X is the smallest closed set containing A.

Definition 9 The *interior* $\mathring{A}$ of a subset A of X is the largest open set contained in A.

Remark It is sometimes useful to define the *boundary* of A as the set $\bar{A} \setminus \mathring{A} = \{x \in \bar{A}, x \notin \mathring{A}\}$.

Definition 10 Let A be a subset of a topological space X. A point $x \in X$ is called a *limit point* of A if every open set containing x contains some point of A other than x.

Definition 11 A subset A of X is said to be *dense* in X if $\bar{A} = X$.

Definition 12 A topological space X is called a *Hausdorff space* if for any two distinct points $x, y \in X$, there exist an open neighborhood of A of x and an open neighborhood B of y such that A and B are disjoint (that is, $A \cap B = \emptyset$).

Remark and Examples

(i) This is looking more like what we expect. However, certain mildly non-Hausdorff spaces turn out to be quite useful, for example, in twistor theory. A "pocket" furnishes such an example. Explicitly, consider X to be the subset of the real plane consisting of the interval $[-1, 1]$ on the x-axis, together with the interval $[0, 1]$ on the line $y = 1$, where the following pairs of points are identified: $(x, 0) \cong (x, 1), 0 < x \leq 1$. Then the two points $(0, 0)$ and $(0, 1)$ do not have any disjoint neighborhoods. Strictly speaking, one needs the notion of a quotient topology, introduced below.

(ii) For a more "truly" non-Hausdorff topology, consider the space of positive integers $\mathbb{N} = \{1, 2, 3, \ldots\}$, and take as open sets the following: $\emptyset$, $\mathbb{N}$, and the sets $\{1, 2, \ldots, n\}$ for each $n \in \mathbb{N}$. This space is neither Hausdorff nor compact (see later for definition of compactness).

Definition 13 Let X and Y be two topological spaces and let $f : X \to Y$ be a map from X to Y. We say that f is *continuous* if $f^{-1}(A)$ is open (in X) whenever A is open (in Y).

Remark Continuity is the single most important concept here. In this general setting, it looks a little different from the "ϵ–δ" definition, but this latter works only for metric spaces, which we shall come to shortly.

Definition 14 A map $f : X \to Y$ is a *homeomorphism* if it is a continuous bijective map such that its inverse f^{-1} is also continuous.

Remark Homeomorphisms are the natural maps for topological spaces, in the sense that two homeomorphic spaces are "indistinguishable" from the point of view of topology. Topological invariants are properties of topological spaces which are preserved under homeomorphisms.

Definition 15 Let $B \subseteq A$. Then one can define the *relative topology* of B by saying that a subset $C \subseteq B$ is open if and only if there exists an open set D of A such that $C = D \cap B$.

Definition 16 A subset $B \subseteq A$ equipped with the relative topology is called a *subspace* of the topological space A.

Remark Thus, if for subsets of the real line, we consider $A = [0, 3], B = [0, 2]$, then $C = (1, 2]$ is open in B, in the relative topology induced by the usual topology of $\mathbb{R}$.

Definition 17 Given two topological spaces X and Y, we can define a *product topological space* $Z = X \times Y$, where the set is the Cartesian product of the two sets X and Y, and sets of the form $A \times B$, where A is open in X and B is open in Y, form a basis for the topology.

Remark Note that the open sets of $X \times Y$ are not always of this product form $(A \times B)$.

Definition 18 Suppose there is a partition of X into disjoint subsets $A_\alpha, \alpha \in \mathcal{I}$, for some index set $\mathcal{I}$, or equivalently, there is defined on X an equivalence relation $\sim$. Then one can define the *quotient topology* on the set of equivalence classes $\{A_\alpha, \alpha \in \mathcal{I}\}$, usually denoted as the quotient space $X/\sim = Y$, as follows. Consider the map $\pi : X \to Y$, called the canonical projection, which maps the element $x \in X$ to its equivalence class $[x]$. Then a subset $U \subseteq Y$ is open if and only if $\pi^{-1}(U)$ is open.

Proposition 1 *Let $\mathcal{T}$ be the quotient topology on the quotient space Y. Suppose $\mathcal{T}'$ is another*

topology on Y such that the canonical projection is continuous, then $\mathcal{T}' \subseteq \mathcal{T}$.

Definition 19 An *(open) cover* $\{U_\alpha : \alpha \in \mathcal{I}\}$ for X is a collection of open sets $U_\alpha \subseteq X$ such that their union equals X. A subcover of this cover is then a subset of the collection which is itself a cover for X.

Definition 20 A topological space X is said to be *compact* if every cover contains a finite subcover.

Remark So for a compact space, however one chooses to cover it, it is always sufficient to use a finite number of open subsets. This is one of the essential differences between an open interval (not compact) and a closed interval (compact). The former is in fact homeomorphic to the entire real line.

Definition 21 A topological space X is said to be *connected* if it cannot be written as the union of two nonempty disjoint open sets.

Remark A useful equivalent definition is that any continuous map from X to the two-point set $\{0, 1\}$, equipped with the discrete topology, cannot be surjective.

Definition 22 Given two points x, y in a topological space X, a *path* from x to y is a continuous map $f : [0, 1] \to X$ such that $f(0) = x, f(1) = y$. We also say that such a path joins x and y.

Definition 23 A topological space X is *path-connected* if every two points in X can be joined by a path lying entirely in X.

Proposition 2 *A path-connected space is connected.*

Proposition 3 *A connected open subspace of $\mathbb{R}^n$ is path-connected.*

Definition 24 Given a topological space X, define an equivalence relation by saying that $x \sim y$ if and only if x and y belong to the same connected subspace of X. Then the equivalence classes are called *(connected) components* of X.

Examples

(i) The Lie group O(3) of 3×3 orthogonal matrices has two connected components. The identity connected component is SO(3) and is a subgroup.
(ii) The proper orthochronous Lorentz transformations of Minkowski space form the identity component of the group of Lorentz transformations.

Metric Spaces

A special class of topological spaces plays an important role: metric spaces.

Definition 25 A *metric space* is a set X together with a function $d : X \times X \to \mathbb{R}$ satisfying

(i) $d(x, y) \geq 0$,
(ii) $d(x, y) = 0 \Leftrightarrow x = y$,
(iii) $d(x, z) \leq d(x, y) + d(y, z)$ ("triangle inequality").

Remarks

(i) The function d is called the metric, or distance function, between the two points.
(ii) This concept of metric is what is generally known as "Euclidean" metric in mathematical physics. The distinguishing feature is the positive definiteness (and the triangle inequality). One can, and does, introduce indefinite metrics (for example, the Minkowski metric) with various signatures. But these metrics are not usually used to induce topologies in the spaces concerned.

Definition 26 Given a metric space X and a point $x \in X$, we define the *open ball* centred at x with radius r (a positive real number) as

$$B_r(x) = \{y \in X : d(x, y) < r\}$$

Given a metric space X, we can immediately define a topology on it by taking all the open balls in X as a basis. We say that this is the topology induced by the given metric. Then we can recover our usual "ϵ–δ" definition of continuity.

Proposition 4 *Let $f : X \to Y$ be a map from the metric space X to the metric space Y. Then f is continuous (with respect to the corresponding induced topologies) at $x \in X$ if and only if given any $\epsilon > 0, \exists \delta > 0$ such that $d(x, x') < \delta$ implies $d(f(x,), f(x')) < \epsilon$.*

Note that we do not bother to give two different symbols to the two metrics, as it is clear which spaces are involved. The proof is easily seen by taking the relevant balls as neighborhoods. Equally easy is the following:

Proposition 5 *A metric space is Hausdorff.*

Definition 27 A map $f : X \to Y$ of metric spaces is *uniformly continuous* if given any $\epsilon > 0$ there exists $\delta > 0$ such that for any $x_1, x_2 \in X, d(x_1, x_2) < \delta$ implies $d(f(x_1), f(x_2)) < \epsilon$.

Remark Note the difference between continuity and uniform continuity: the latter is stronger and requires the same δ for the whole space.

Definition 28 Two metrics d_1 and d_2 defined on X are *equivalent* if there exist positive constants a and b such that for any two points $x, y \in X$ we have

$$a d_1(x, y) \leq d_2(x, y) \leq b d_1(x, y)$$

Remark This is clearly an equivalence relation. Two equivalent metrics induce the same topology.

Examples

(i) Given a set X, we can define the discrete metric as follows: $d_0(x,y)=1$ whenever $x \neq y$. This induces the discrete topology on X. This is quite a convenient way of describing the discrete topology.

(ii) In $\mathbb{R}$, the usual metric is $d(x,y)=|x-y|$, and the usual topology is the one induced by this.

(iii) More generally, in $\mathbb{R}^n$, we can define a metric for every $p \geq 1$ by

$$d_p(x,y) = \left\{ \sum_{k=1}^{n} |x_k - y_k|^p \right\}^{1/p}$$

where $x=(x_1,x_2,\ldots,x_n), y=(y_1,y_2,\ldots,y_n)$. In particular, for $p=2$ we have the usual Euclidean metric, but the other cases are also useful. To continue the series, one can define

$$d_\infty = \max_{1<k<n} \{|x_k - y_k|\}$$

All these metrics induce the same topology on $\mathbb{R}^n$.

(iv) In a vector space V, say over the real or the complex field, a function $\|\cdot\| : V \to \mathbb{R}^+$ is called a *norm* if it satisfies the following axioms:
(a) $\|x\|=0$ if and only if $x=0$,
(b) $\|\alpha x\| = |\alpha| \|x\|$, and
(c) $\|x+y\| \leq \|x\| + \|y\|$.

Then it is easy to see that a metric can be defined using the norm

$$d(x,y) = \|x-y\|$$

In many cases, for example, the metrics defined in example (iii) above, one can define the norm of a vector as just the distance of it from the origin. One obvious exception is the discrete metric.

A slightly more general concept is found to be useful for spaces of functions and operators: that of seminorms. A *seminorm* is one which satisfies the last two of the conditions, but not necessarily the first, for a norm, as listed above.

Definition 29 Given a metric space X, a sequence of points $\{x_1,x_2,\ldots\}$ is called a *Cauchy sequence* if, given any $\epsilon > 0$, there exists a positive integer N such that for any $k,\ell > N$ we have $d(x_k,x_\ell) < \epsilon$.

Definition 30 Given a sequence of points $\{x_1,x_2,\ldots\}$ in a metric space X, a point $x \in X$ is called a *limit* of the sequence if given any $\epsilon > 0$, there exists a positive integer N such that for any $n > N$ we have $d(x,x_n) < \epsilon$. We say that the sequence *converges* to x.

Definition 31 A metric space X is *complete* if every Cauchy sequence in X converges to a limit in it.

Examples

(i) The closed interval $[0,1]$ on the real line is complete, whereas the open interval $(0,1)$ is not. For example, the Cauchy sequence $\{1/n, n=2,3,\ldots\}$ has no limit in this open interval. (Considered as a sequence on the real line, it has of course the limit point 0.)

(ii) The spaces $\mathbb{R}^n$ are complete.

(iii) The Hilbert space ℓ^2 consisting of all sequences of real numbers $\{x_1,x_2,\ldots\}$ such that $\sum_1^\infty x_k^2$ converges is complete with respect to the obvious metric which is a generalization to infinite dimension of d_2 above. For arbitrary $p \geq 1$, one can similarly define ℓ^p, which are also complete and are hence Banach spaces.

Remarks Completeness is not a topological invariant. For example, the open interval $(-1,1)$ and the whole real line are homeomorphic (with respect to the usual topologies) but the former is not complete while the latter is. The homeomorphism can conveniently be given in terms of the trigonometric function tangent.

Definition 32 A subset B of the metric space X is *bounded* if there exists a ball of radius R $(R>0)$ which contains it entirely.

Theorem 1 (Heine–Borel) *Any closed bounded subset of* $\mathbb{R}^n$ *is compact.*

Remark The converse is also true. We have thus a nice characterization of compact subsets of $\mathbb{R}^n$ as being closed and bounded.

Proposition 6 *Any bounded sequence in* $\mathbb{R}^n$ *has a convergent subsequence.*

Definition 33 Consider a sequence $\{f_n\}$ of real-valued functions on a subset A (usually an interval) of $\mathbb{R}$. We say that $\{f_n\}$ *converges pointwise* in A if the sequence of real numbers $\{f_n(x)\}$ converges for every $x \in A$. We can then define a function $f : A \to \mathbb{R}$ by $f(x) = \lim_{n\to\infty} f_n(x)$, and write $f_n \to f$.

Definition 34 A sequence of functions $f_n : A \to \mathbb{R}, A \subseteq \mathbb{R}$ is said to *converge uniformly* to a function $f : A \to \mathbb{R}$ if given any $\epsilon > 0$, there exists a positive integer N such that, for all x, $|f_n(x) - f(x)| < \epsilon$ whenever $n > N$.

Theorem 2 *Let* $f_n : (a,b) \to \mathbb{R}$ *be a sequence of functions continuous at the point* $c \in (a,b)$, *and suppose* f_n *converges uniformly to* f *on* (a,b). *Then* f *is continuous at* c.

Remark and Example The pointwise limit of continuous functions need not be continuous, as can be shown by the following example: $f_n(x) = x^n, x \in [0,1]$. We see that the limit function f is not continuous:

$$f(x) = \begin{cases} 0 & x \neq 1 \\ 1 & x = 1 \end{cases}$$

Definition 35 Let X be a metric space. A map $f: X \to X$ is a *contraction* if there exists $c < 1$ such that $d(f(x), f(y)) \leq cd(x, y)$ for all $x, y \in X$.

Theorem 3 (Banach) *If X is a complete metric space and f is a contraction in X, then f has a unique fixed point $x \in X$, that is, $f(x) = x$.*

Some Function and Operator Spaces

The spaces of functions and operators can be equipped with different topologies, given by various concepts of convergence and of norms (or sometimes seminorms), very often with different such concepts for the same space. As we saw earlier, a norm in a vector space gives rise to a metric, and hence to a topology. Similarly with the concept of convergence for sequences of functions and operators, as one then knows what the limit points, and hence closed sets, are.

But before we do that, let us introduce, in a slightly different context, a topology which is in some sense the natural one for the space of continuous maps from one space to another.

Definition 36 Consider a family F of maps from a topological space X to a topological space Y, and define $W(K, U) = \{f : f \in F, f(K) \subseteq U\}$. Then the family of all sets of the form $W(K, U)$ with K compact (in X) and U open (in Y) form a sub-basis for the *compact open topology* for F.

Consider a topological space X and sequences of functions (f_n) on it. Let $D \subseteq X$. We can then define pointwise convergence and uniform convergence exactly as for functions on subsets of the real line.

Definition 37 Let X, D and (f_n) as above.

(i) The functions f_n *converge pointwise* on D to a function f if the sequence of numbers $f_n(x) \to f(x), \forall x \in D$.
(ii) The functions f_n *converge uniformly* on D to a function f if given $\epsilon > 0$, there exists N such that for all $n > N$ we have $|f_n(x) - f(x)| < \epsilon, \forall x \in D$.

Next we consider the Lebesgue spaces L^p, that is, functions f defined on subsets of $\mathbb{R}^n$, such that $|f(x)|^p$ is Lebesgue integrable, for real numbers $p \geq 1$. To define these spaces, we tacitly take equivalence classes of functions which are equal almost everywhere (that is, up to a null set), but very often we can take representatives of these classes and just deal with genuine functions instead. Note that of all L^p, only L^2 is a Hilbert space.

Definition 38 In the space L^p, we define its norm by

$$\|f\| = \left(\int |f(x)|^p \, dx \right)^{1/p}$$

Now we turn to general normed spaces, and operators on them.

Definition 39 Convergence in the norm is also called strong convergence. In other words, a sequence (x_n) in a normed space X is said to *converge strongly* to x if

$$\lim_{n \to \infty} \|x_n - x\| = 0$$

Definition 40 A sequence (x_n) in a normed space X is said to *converge weakly* to x if

$$\lim_{n \to \infty} f(x_n) = f(x)$$

for all bounded linear functionals f.

Consider the space $B(X, Y)$ of bounded linear operators T from X to Y. We can make this into a normed space by defining the following norm:

$$\|T\| = \sup_{x \in X,\ \|x\| = 1} \|Tx\|$$

Then we can define three different concepts of convergence on $B(X, Y)$. There are in fact more in current use in functional analysis.

Definition 41 Let X and Y be normed spaces and let (T_n) be a sequence of operators $T_n \in B(X, Y)$.

(i) (T_n) is *uniformly convergent* if it converges in the norm.
(ii) (T_n) is *strongly convergent* if $(T_n x)$ converges strongly for every $x \in X$.
(iii) (T_n) is *weakly convergent* if $(T_n x)$ converges weakly for every $x \in X$.

Remark Clearly we have: uniform convergence $\Longrightarrow$ strong convergence $\Longrightarrow$ weak convergence, and the limits are the same in all three cases. However, the converses are in general not true.

Homotopy Groups

The most elementary and obvious property of a topological space X is the number of connected components it has. The next such property, in a certain sense, is the number of holes X has. There

are higher analogues of these, called the *homotopy groups*, which are topological invariants, that is, they are invariant under homeomorphisms. They play important roles in many topological considerations in field theory and other topics of mathematical physics. The articles Topological Defects and Their Homotopy Classification and Electric-Magnetic Duality contain some examples.

Definition 42 Given a topological space X, the zeroth homotopy set, denoted $\pi_0(X)$, is the set of connected components of X. One sometimes writes $\pi_0(X) = 0$ if X is connected.

To define the fundamental group of X, or $\pi_1(X)$, we shall need the concept of closed loops, which we shall find useful in other ways too. For simplicity, we shall consider based loops (that is, loops passing through a fixed point in X). It seems that in most applications, these are the relevant ones. One could consider loops of various smoothness (when X is a manifold), but in view of applications to quantum field theory, we shall consider continuous loops, which are also the ones relevant for topology.

Definition 43 Given a topological space X and a point $x_0 \in X$, a (*closed*) (*based*) *loop* is a continuous function of the parametrized circle to X:

$$\xi : [0, 2\pi] \to X$$

satisfying $\xi(0) = \xi(2\pi) = x_0$.

Definition 44 Given a connected topological space X and a point $x_0 \in X$, the space of all closed based loops is called the (parametrized based) *loop space* of X, denoted ΩX.

Remarks

(i) The loop space ΩX inherits the relative compact–open topology from the space of continuous maps from the closed interval $[0, 2\pi]$ to X. It also has a natural base point: the constant function mapping all of $[0, 2\pi]$ to x_0. Hence it is easy to iterate the construction and define $\Omega^k X, k \geq 1$.

(ii) Here we have chosen to parametrize the circle by $[0, 2\pi]$, as is more natural if we think in terms of the phase angle. We could easily have chosen the unit interval [0,1] instead. This would perhaps harmonize better with our previous definition of paths and the definitions of homotopies below.

Proposition 7 *The fundamental group of a topological space X, denoted $\pi_1(X)$, consists of classes of closed loops in X which cannot be continuously deformed into one another while preserving the base point.*

Definition 45 A space X is called *simply connected* if $\pi_1(X)$ is trivial.

To define the higher homotopy groups, let us go into a little detail about homotopy.

Definition 46 Given two topological spaces X and Y, and maps

$$p, q : X \to Y$$

we say that h is a *homotopy* between the maps p, q if

$$h : X \times I \to Y$$

is a continuous map such that $h(x, 0) = p(x)$, $h(x, 1) = q(x)$, where I is the unit interval $[0, 1]$. In this case, we write $p \simeq q$.

Definition 47 A map $f : X \to Y$ is a *homotopy equivalence* if there exists a map $g : Y \to X$ such that $g \circ f \simeq \mathrm{id}_X$ and $f \circ g \simeq \mathrm{id}_Y$.

Remark This is an equivalence relation.

Definition 48 For a topological space X with base point x_0, we define $\pi_n(X), n \geq 0$ as the set of homotopy equivalence classes of based maps from the n-sphere S^n to X.

Remark This coincides with the previous definitions for π_0 and π_1.

There is a very nice relation between homotopy classes and loop spaces.

Proposition 8 $\pi_n(X) = \pi_{n-1}(\Omega X) = \cdots = \pi_0(\Omega^n X)$.

Remarks

(i) When we consider the gauge group G in a Yang–Mills theory, its fundamental group classifies the monopoles that can occur in the theory.

(ii) For $n \geq 1, \pi_n(X)$ is a group, the group action coming from the joining of two loops together to form a new loop. On the other hand, $\pi_0(X)$ in general is not a group. However, when X is a Lie group, then $\pi_0(X)$ inherits a group structure from X, because it can be identified with the quotient group of X by its identity-connected component. For example, the two components of O(3) can be identified with the two elements of the group $\mathbb{Z}_2$, the component where the determinant equals 1 corresponding to 0 in $\mathbb{Z}_2$ and the component where the determinant equals -1 corresponding to 1 in $\mathbb{Z}_2$.

(iii) For $n \geq 2$, the group $\pi_n(X)$ is always abelian.

(iv) Examples of nonabelian π_1 are the fundamental groups of some Riemann surfaces.

(v) Since π_1 is not necessarily abelian, much of the direct-sum notation we use for the homotopy

groups should more correctly be written multiplicatively. However, in most literature in mathematical physics, the additive notation seems to be preferred.

Examples

(i) $\pi_n(X \times Y) = \pi_n(X) + \pi_n(Y)$, $n \geq 1$.
(ii) For the spheres, we have the following results:

$$\pi_i(S^n) = \begin{cases} 0 & \text{if } i > n \\ \mathbb{Z} & \text{if } i = n \end{cases}$$
$$\pi_i(S^1) = 0 \quad \text{if } i > 1$$
$$\pi_{n+1}(S^n) = \mathbb{Z}_2 \quad \text{if } n \geq 3$$
$$\pi_{n+2}(S^n) = \mathbb{Z}_2 \quad \text{if } n \geq 2$$
$$\pi_6(S^3) = \mathbb{Z}_{12}$$

(iii) From the theory of sphere bundles, we can deduce:

$$\pi_i(S^2) = \pi_{i-1}(S^1) + \pi_i(S^3) \quad \text{if } i \geq 2$$
$$\pi_i(S^4) = \pi_{i-1}(S^3) + \pi_i(S^7) \quad \text{if } i \geq 2$$
$$\pi_i(S^8) = \pi_{i-1}(S^7) + \pi_i(S^{15}) \quad \text{if } i \geq 2$$

and the first of these relations give the following more succinct result:

$$\pi_i(S^3) = \pi_i(S^2) \quad \text{if } i \geq 3$$

(iv) A result of Serre says that all the homotopy groups of spheres are in fact finite except $\pi_n(S^n)$ and $\pi_{4n-1}(S^{2n})$, $n \geq 1$.

Definition 49 Given a connected space X, a map $\pi : B \to X$ is called a *covering* if (i) $\pi(B) = X$, and (ii) for each $x \in X$, there exists an open connected neighborhood V of x such that each component of $\pi^{-1}(V)$ is open in B, and π restricted to each component is a homeomorphism. The space B is called a *covering space*.

Examples

(i) The real line $\mathbb{R}$ is a covering of the group U(1).
(ii) The group SU(2) is a double cover of the group SO(3).
(iii) The group SL(2, $\mathbb{C}$) is a double cover of the Lorentz group SO(1, 3).
(iv) The group SU(2, 2) is a 4-fold cover of the conformal group in four dimensions. This local isomorphism is of great importance in twistor theory.

Remarks

(i) By considering closed loops in X and their coverings in B it is easily seen that the fundamental group $\pi_1(X)$ acts on the coverings of X. If we further assume that the action is transitive, then we have the following nice result: coverings of X are in 1–1 correspondence with normal subgroups of $\pi_1(X)$.
(ii) Given a connected space X, there always exists a unique connected simply connected covering space $\widetilde{X}$, called the universal covering space. Furthermore, $\widetilde{X}$ covers all the other covering spaces of X. For the higher homotopy groups, one has

$$\pi_n(X) = \pi_n(\widetilde{X}), \quad n \geq 2$$

One very important class of homotopy groups are those of Lie groups. To simplify matters, we shall consider only connected groups, that is, $\pi_0(G) = 0$. Also we shall deal mainly with the classical groups, and in particular, the orthogonal and unitary groups.

Proposition 9 *Suppose that G is a connected Lie group.*

(i) *If G is compact and semi-simple, then $\pi_1(G)$ is finite. This implies that $\widetilde{G}$ is still compact.*
(ii) $\pi_2(G) = 0$.
(iii) *For G compact, simple, and nonabelian,* $\pi_3(G) = \mathbb{Z}$.
(iv) *For G compact, simply connected, and simple,* $\pi_4(G) = 0$ or $\mathbb{Z}_2$.

Examples

(i) $\pi_1(\mathrm{SU}(n)) = 0$.
(ii) $\pi_1(\mathrm{SO}(n)) = \mathbb{Z}_2$.
(iii) Since the unitary groups U(n) are topologically the product of SU(n) with a circle S^1, their homotopy groups are easily computed using the product formula. We remind ourselves that U(1) is topologically a circle and SU(2) topologically S^3.
(iv) For $i \geq 2$, we have:

$$\pi_i(\mathrm{SO}(3)) = \pi_i(\mathrm{SU}(2))$$
$$\pi_i(\mathrm{SO}(5)) = \pi_i(\mathrm{Sp}(2))$$
$$\pi_i(\mathrm{SO}(6)) = \pi_i(\mathrm{SU}(4))$$

Just for interest, and to show the richness of the subject, some isomorphisms for homotopy groups are shown in **Table 1** and some homotopy groups for low SU(n) and SO(n) are listed in **Table 2**.

Table 1 Some isomorphisms for homotopy groups

Isomorphism	*Range*
$\pi_i(\mathrm{SO}(n)) \cong \pi_i(\mathrm{SO}(m))$	$n, m \geq i + 2$
$\pi_i(\mathrm{SU}(n)) \cong \pi_i(\mathrm{SU}(m))$	$n, m \geq \frac{1}{2}(i + 1)$
$\pi_i(\mathrm{Sp}(n)) \cong \pi_i(\mathrm{Sp}(m))$	$n, m \geq \frac{1}{4}(i - 1)$
$\pi_i(G_2) \cong \pi_i(\mathrm{SO}(7))$	$2 \leq i \leq 5$
$\pi_i(F_4) \cong \pi_i(\mathrm{SO}(9))$	$2 \leq i \leq 6$
$\pi_i(\mathrm{SO}(9)) \cong \pi_i(\mathrm{SO}(7))$	$i \leq 13$

Table 2 Some homotopy groups for low SU(n) and SO(n)

	π_4	π_5	π_6	π_7	π_8	π_9	π_{10}
SU(2)	Z_2	Z_2	Z_{12}	Z_2	Z_2	Z_3	Z_{15}
SU(3)	0	Z	Z_6	0	Z_{12}	Z_3	Z_{30}
SU(4)	0	Z	0	Z	Z_{24}	Z_2	$Z_{120}+Z_2$
SU(5)	0	Z	0	Z	0	Z	Z_{120}
SU(6)	0	Z	0	Z	0	Z	Z_3
SO(5)	Z_2	Z_2	0	Z	0	0	Z_{120}
SO(6)	0	Z	0	Z	Z_{24}	Z_2	$Z_{120}+Z_2$
SO(7)	0	0	0	Z	Z_2+Z_2	Z_2+Z_2	Z_{24}
SO(8)	0	0	0	$Z+Z$	$Z_2+Z_2+Z_2$	$Z_2+Z_2+Z_2$	$Z_{24}+Z_{24}$
SO(9)	0	0	0	Z	Z_2+Z_2	Z_2+Z_2	Z_{24}
SO(10)	0	0	0	Z	Z_2	$Z+Z_2$	Z_{12}

Appendix: A Mathematician's Basic Toolkit

The following is a drastically condensed list, most of which is what a mathematics undergraduate learns in the first few weeks. The rest is included for easy reference. These notations and concepts are used universally in mathematical writing. We have not endeavored to arrange the material in a logical order. Furthermore, given structures such as sets, groups, etc., one can usually define "substructures" such as subsets, subgroups, etc., in a straightforward manner. We shall therefore not spell this out.

Sets

$A \cup B = \{x : x \in A \text{ or } x \in B\}$ union

$A \cap B = \{x : x \in A \text{ and } x \in B\}$ intersection

$A \backslash B = \{x : x \in A \text{ and } x \notin B\}$ complement

$A \times B = \{(x, y) : x \in A, y \in B\}$ Cartesian product

Maps

1. A map or mapping $f : A \to B$ is an assignment of an element $f(x)$ of B for every $x \in A$.
2. A map $f : A \to B$ is injective if $f(x) = f(y) \Longrightarrow x = y$. This is sometimes called a 1–1 map, a term to be avoided.
3. A map $f : A \to B$ is surjective if for every $y \in B$ there exists an $x \in A$ such that $y = f(x)$. This is sometimes called an "onto" map.
4. A map $f : A \to B$ is bijective if it is both surjective and injective. This is also sometimes called a 1–1 map, a term to be equally avoided.
5. For any map $f : A \to B$ and any subset $C \subseteq B$, the inverse image $f^{-1}(C) = \{x : f(x) \in C\} \subseteq A$ is always defined, although, of course, it can be empty. On the other hand, the map f^{-1} is defined if and only if f is bijective.
6. A map from a set to either the real or complex numbers is usually called a function.
7. A map between vector spaces, and more particularly normed spaces (including Hilbert spaces), is called an operator. Most often, one considers linear operators.
8. An operator from a vector space to its field of scalars is called a functional. Again, one considers almost exclusively linear functionals.

Relations

1. A relation $\sim$ on a set A is a subset $R \subseteq A \times A$. We say that $x \sim y$ if $(x, y) \in R$.
2. We shall only be interested in equivalence relations. An equivalence relation $\sim$ is one satisfying, for all $x, y, z \in A$:
   (a) $x \sim x$ ("reflexive"),
   (b) $x \sim y \Longrightarrow y \sim x$ ("symmetric"),
   (c) $x \sim y, y \sim z \Longrightarrow x \sim z$ ("transitive").
3. If $\sim$ is an equivalence relation in A, then for each $x \in A$, we can define its equivalence class:

$$[x] = \{y \in A : y \sim x\}$$

   It can be shown that equivalence classes are nonempty, any two equivalence classes are either equal or disjoint, and they together partition the set A. Subgroup equivalence classes are called cosets.
4. An element of an equivalence class is called a representative.

Groups

A group is a set G with a map, called multiplication or group law

$$G \times G \longrightarrow G$$
$$(x, y) \longmapsto xy$$

satisfying

1. $(xy)z = x(yz), \forall x, y, z \in G$ ("associative");
2. there exists a neutral element (or identity) 1 such that $1x = x1 = x, \forall x \in G$; and
3. every element $x \in G$ has an inverse x^{-1}, that is, $xx^{-1} = x^{-1}x = 1$.

A map such as the multiplication in the definition is an example of a binary operation. Note that we have denoted the group law as multiplication here. It is usual to denote it additively if the group is abelian, that is, if $xy = yx, \forall x, y \in G$. In this case, we may write the condition as $x + y = y + x$, and call the identity element 0.

Rings

A ring is a set R equipped with two binary operations, $x + y$ called addition, and xy called multiplication, such that

1. R is an abelian group under addition;
2. the multiplication is associative; and
3. $(x + y)z = xz + yz, x(y + z) = xy + xz, \forall x, y, z \in R$ ("distributive").

If the multiplication is commutative ($xy = yx$) then the ring is said to be commutative. A ring may contain a multiplicative identity, in which case it is called a ring with unit element.

An ideal I of R is a subring of R, satisfying in addition

$$r \in R, a \in I \Longrightarrow ra \in I, ar \in I$$

One can define in an obvious fashion a left-ideal and a right- ideal. The above definition will then be for a two-sided ideal.

Modules

Given a ring R, an R-module is an abelian group M, together with an operation, $M \times R \to M$, denoted multiplicatively, satisfying, for $x, y \in M, r, s \in R$,

1. $(x + y)r = xr + yr$,
2. $x(r + s) = xr + xs$,
3. $x(rs) = (xr)s$, and
4. $x1 = x$

The term right R-module is sometimes used, to distinguish it from obviously defined left R-modules.

Fields

A field F is a commutative ring in which every nonzero element is invertible.

The additive identity 0 is never invertible, unless $0 = 1$, so it is usual to assume that a field has at least two elements, 0 and 1.

The most common fields we come across are, of course, the number fields: the rationals, the reals, and the complex numbers.

Vector Spaces

A vector space, or sometimes linear space, V, over a field F, is an abelian group, written additively, with a map $F \times V \to V$ such that, for $x, y \in V, \alpha, \beta \in F$,

1. $\alpha(x + y) = \alpha x + \alpha y$ ("linearity"),
2. $(\alpha + \beta)x = \alpha x + \beta x$,
3. $(\alpha\beta)x = \alpha(\beta x)$, and
4. $1x = x$.

A vector space is then a right (or left) F-module. The elements of V are called vectors, and those of F scalars.

Algebras

An algebra A over a field F is a ring which is a vector space over F, such that

$$\alpha(ab) = (\alpha a)b = a(\alpha b), \quad \alpha \in F, \ a, b \in A$$

Note that in some older literature, particularly the Russian school, an algebra of operators is called a ring of operators.

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（穆良柱 译 陈熙谋 校）

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