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Lecture Notes of Quantum Mechanics

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Lecture Notes 1 Review of Classical Mechanics

Contents

- Castesian (Descartes, 笛卡尔) coordinates and Euclidean space (3-dimensional);
- Newtonian Mechanics, Lagrangian Mechanics, Hamiltonian Mechanics;
- Charged Paricles in Electromagnetic Field.

Castesian/Descartes coordinates and Euclidean space (3-dimensional)

1. Coordinate system: rectangular coordinate system; cyclindrical coordinate system; spherical coordinate system. (直角/柱/球坐标系)
2. Inertial frame and non-inertial frame. (惯性系与非惯性系)
3. Mass point system (质点系) and point mass (and system of particles, or mass points, 质点); and rigid body (刚体).
4. Inertia (惯性): mass m and inertia of rotation mr^2.

Dynamics of Newtonian Mechanics

Momentum and Force	Angular Momentum and Torque
$\dfrac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \boldsymbol{F}$	$\dfrac{\mathrm{d}\boldsymbol{L}}{\mathrm{d}t} = \boldsymbol{N}$
$\boldsymbol{p} = m\boldsymbol{v}$	$\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}$, $\boldsymbol{N} = \boldsymbol{x} \times \boldsymbol{F}$

Lagrangian Mechanics

1. Constraint System (holonomic and non-holonomic): $x_1, x_2, \cdots, x_{3N}$ are not independent.
2. Generalized coordinates (position and velocity): $x_1, x_2, \cdots, x_{3N} \rightarrow q_1, q_2, \cdots, q_{3N}$ are independent.
3. Spaces: (see the table below)
4. Scalar equations in Lagrangian Mechanics (LM).

   The numbers of equations of LM $\leq$ The numbers of Newtonian Mechanics.

Physical Space (Kinetic)	Configuration Space (Abstract)
$\boldsymbol{x}(t)$	$q(t)$
$3N$-dimensional	D-dimensional ($D \leq 3N$)

5. On constraints: holonomic constraint and non-holonomic constraint (完整约束与非完整约束).

   holonomic: $f(x_i; t) = 0$; non-holonomic: $g(x_i, \dot{x}; t) = 0$.

   The only concern involved in the courses of non-holonomic constraint is charged particle in EM field.

6. Dimensions (量纲) of generalized coordinates (position or velocity) do not need to be the same as position (or velocity): e.g., curvilinear coordinates (cylindrical, spherical) do not necessarily have the dimensions or "length".

7. Action (作用量):
$$S[q] = \int_{t_1}^{t_2} L(q(t), \dot{q}(t); t)\mathrm{dt}.$$

8. Principle of Least Action (Hamiltonian principle, 最小作用量原理, Hamilton 原理):
$$\delta S[q] = 0 \Rightarrow q(t), \quad \text{to make } S = S_{\text{extreme}}.$$

9. Derivation of Euler-Lagrange's equation:
$$\frac{\mathrm{d}}{\mathrm{dt}}\left(\frac{\partial L}{\partial \dot{q}_a}\right) = \frac{\partial L}{\partial q_a}, \quad (a = 1, 2, \cdots D).$$

   2^{nd}-order differential equations, with the total number of D.

10. Applications:
$$\text{Lagrangian Mechanics} \Rightarrow \begin{cases} \text{Lagrangian-based Quantum Mechanics} \\ \text{Path-integral in Quantum Mechanics} \\ \Downarrow \\ \text{Relativistic QM and QFT (gauge field theory)} \end{cases}$$

Hamiltonian Mechanics

1. Legendre Transformation and canonical coordinates (position/momentum):

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \Rightarrow H(q,p;t) = \sum_i p_i \dot{q}_i - L(q,\dot{q};t).$$

p_i: canonical momentum; generalized momentum; conjugate variable of canonical position (正则动量；广义动量；正则位置的共轭量).

$$\underbrace{L(q,\dot{q};t)}_{\text{no p (momentum)}} \rightarrow \underbrace{H(q,p;t)}_{\text{no } \dot{q} \text{ (velocity)}}$$

Hamiltonian canonical equations of motion:

$$\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}; \quad \dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}.$$

Generalized equation for $\forall\ f(q,p;t)$:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + [f,H]_{PB},$$

where PB denotes the Poissonian Bracket (Classical Canonical Commutator, 泊松括号, 或经典正则对易子)

$$[f,H]_{\mathrm{PB}} = \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i}\right) = \sum_i \left(\frac{\partial f}{\partial q_i}\dot{q}_i + \frac{\partial f}{\partial p_i}\dot{p}_i\right).$$

2. Phase Space (相空间, abstract space):

configuration space	$\rightarrow$	phase space
$q(t)$	$\rightarrow$	$q(t), p(t)$
D-dimensional	$\rightarrow$	$2D$-dimensional

Phase Space Transformation (Canonical Transformation, 正则变换):

Four types of generating functions to accomplish the canonical transformation:

$$\left[\sum_i p_i \mathrm{d}q_i - H(q,p;t)\right] - \left[\sum_i P_i \mathrm{d}Q_i - K(Q,P;t)\right] = \underbrace{\mathrm{d}G}_{\text{generating function}}.$$

There are 4 types of generating functions G:

$H(q,p;t)$	$\to$	$K(Q,P;t)$	unchanged
$\begin{cases}\dot{q}_i=\dfrac{\partial H}{\partial p_i},\\ \dot{p}_i=-\dfrac{\partial H}{\partial q_i}.\end{cases}$	$\to$	$\begin{cases}\dot{Q}_i=\dfrac{\partial H}{\partial P_i},\\ \dot{P}_i=-\dfrac{\partial H}{\partial Q_i}.\end{cases}$	canonical equations of motion
$\begin{cases}[q_i,p_j]_{PB}=\delta_{ij},\\ [q_i,q_j]_{PB}=[p_i,p_j]_{PB}\equiv 0.\end{cases}$	$\to$	$\begin{cases}[Q_i,P_j]_{PB}=\delta_{ij},\\ [Q_i,Q_j]_{PB}=[P_i,P_j]_{PB}\equiv 0.\end{cases}$	canonical commutation

  - Type-I: $G_1(q,Q;t)$;
  - Type-II: $G_2(q,P;t)$: $G_1\to G_2$-Legendre Transformation: $Q\ \to\ P$;
  - Type-III: $G_3(p,Q;t)$: $G_1\to G_3$-Legendre Transformation: $q\ \to\ p$;
  - Type-IV: $G_4(p,P;t)$: $G_1\to G_4$-Legendre Transformation: $q\ \to\ p$; $Q\ \to\ P$.

  Canonical: "Right" $\to$ No change (canonical equations of motion; Poisson Bracket, etc.)

3. Dynamics in phase space (q,p):

phase point	$\to$	the concept of "state" (in statistical mechanics)
phase point density	$\to$	$\rho(q,p;t)\Rightarrow\int\rho\mathrm{d}^Dq\mathrm{d}^Dp=1$

- Continuity equation:
$$\frac{\mathrm{d}\rho}{\mathrm{d}t}\equiv 0=\frac{\partial\rho}{\partial t}+[\rho,H]_{PB}.$$
$\Rightarrow$ Liouville's equation:
$$\frac{\partial\rho}{\partial t}=[H,\rho]_{PB}.$$

4. Summary of analytical mechanics:

   Toolbox are ready for Quantum Mechanics!

   Toolbox for QM, offered by CM:

   (1)

$$\underbrace{\text{Hamiltonian}}_{(H=T+V)}\to\text{canonical}\begin{cases}\text{coordinates 坐标}(q,p)\text{(not kinetic physical)}\\ \text{transformations 变换}\\ \Rightarrow\text{unchanged e.g., CCC (classical canonical commutation)}\\ \text{equations of motion 方程}\leftrightarrow\text{Heisenberg's equation}\\ \text{commutation 对易}\end{cases}$$

(2) Comparisons of QM vs. CM.

CM		QM
CCC (classical canonical commutation)		QCC (quantum canonical commutation)
$[A,B]_{PB}$	$\xrightarrow{\text{PCC} \to \text{QCC}}$	$\frac{1}{i\hbar}[\hat{A},\hat{B}]$
$\frac{\mathrm{df}}{\mathrm{dt}} = \frac{\partial f}{\partial t} + [f,H]_{PB}.$	$\xrightarrow{[\ ,\ ]\to 1/i\hbar[\ ,\ ]}$	$\frac{\mathrm{d}\hat{f}}{\mathrm{d}t} = \frac{\partial \hat{f}}{\partial t} + [\hat{f},\hat{H}]_{PB}.$
$\begin{cases}\dot{q} = [q,H]_{PB},\\ \dot{p} = [p,H]_{PB}.\end{cases}$	$\longrightarrow$	$\begin{cases}\dot{\boldsymbol{x}} = \frac{1}{i\hbar}[\hat{\boldsymbol{x}},\hat{H}],\\ \dot{\boldsymbol{p}} = \frac{1}{i\hbar}[\hat{\boldsymbol{p}},H].\end{cases}$
phase point: "state"	$\longrightarrow$	state vector in Hilbert space.

(3) Phase space and the concept of "state" in statistical mechanics;

(4) Hilbert space (function space) theory is almost ready;

(5) Group theory is ready: Abstract group theory; Lie group and Lie algebra;

(6) Vector analysis (algebra + calculus) is ready:

Gibbs; Heaviside; $\cdots \Rightarrow$ Hamiltonian-based Quantum Mechanics (canonical quantization based QM): Non-Relativistic QM.

Charged Paricles in Electromagnetic Field

$$\begin{cases} L = \frac{1}{2}m\dot{\boldsymbol{x}}^2 - q\Phi + \frac{q}{c}\boldsymbol{v}\cdot\boldsymbol{A},\\ H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}\right)^2 + q\phi. \end{cases}$$

Non-holonomic constraint (非完整约束): in this case, one has $U(\boldsymbol{x},\dot{\boldsymbol{x}};t)\equiv 0$, instead of $U(\boldsymbol{x};t)\equiv 0$.

$$\begin{cases} \boldsymbol{p} & : \text{ canonical momentum;}\\ \boldsymbol{p} - \frac{q}{c}\boldsymbol{A} & : \text{ kinetic momentum.} \end{cases}$$

(The above two $\boldsymbol{p}$'s can be derived from d'Alembert's principle, using generalized force.)

Legendre's Transformation

$$f(x) \to g(p) = f(x) - xf'(x) = f(x) - xp \quad \Big(p = f'(x)\Big).$$

Generalized:

$$\begin{aligned} f(x_i, y_j) \to g(x_i, p_j) =& f(x_i, y_j) - \sum_j y_j \frac{\partial f}{\partial y_j} \\ =& f(x_i, y_j) - \sum_j y_j p_j, \end{aligned}$$

where $p_j = \dfrac{\partial f}{\partial y_j}$ has been used to derive the above equation. Therefore one yields

$$\frac{\partial g}{\partial y_j} = \frac{\partial f}{\partial y_j} - p_j = 0.$$

Analogously, one yields

$$\frac{\partial f}{\partial p_j} = \frac{\partial g}{\partial p_j} + y_j = 0, \ \Rightarrow \ y_j = -\frac{\partial g}{\partial p_j}.$$

Hamilton-Jacobi equations:

$$p = \frac{\partial G_1}{\partial q}, \quad P = -\frac{\partial G_1}{\partial Q}, \quad K = H + \frac{\partial G_1}{\partial t}.$$

Let $Q = q_0$, $P = p_0$, $K \equiv 0$, $G_1 = S(q_0, p_0, q, p; t)$, one yields

$$p = \frac{\partial S}{\partial q_0}, \quad p_0 = -\frac{\partial S}{\partial q_0}, \quad \frac{\partial S}{\partial t} = -H\left(q, \frac{\partial S}{\partial q}; t\right).$$

$$\delta S = \frac{\partial L}{\partial \dot{q}} \delta q \Big|_{t_0}^{t} = \begin{cases} \dfrac{\partial L}{\partial \dot{q}} \delta q = p \delta q = \dfrac{\partial S}{\partial q} \delta q \Rightarrow p = \dfrac{\partial S}{\partial q}; \\ -\dfrac{\partial L}{\partial \dot{q}_0} \delta q_0 = -p_0 \delta q_0 = \dfrac{\partial S}{\partial q_0} \delta q_0 \Rightarrow p_0 = -\dfrac{\partial S}{\partial q_0}. \end{cases}$$

$$L = \frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\partial S}{\partial t} + \frac{\partial S}{\partial q} \mathrm{d}q = \frac{\partial S}{\partial t} + p \mathrm{d}q.$$

$$\Rightarrow \frac{\partial S}{\partial t} = -p\mathrm{d}q + L = -(p\mathrm{d}q - L) = -H = -H(q, \frac{\partial S}{\partial q}; t).$$

Classical Mechanics	$\xrightarrow[\text{WKB}]{\text{H−J}}$	Quantum Mechanics
geometric optics	$\to$	wave optics

Exercises:

1. What kind of constraints can (or cannot) be solved by analytical mechanics methods?

2. Use Legendre's Transformation to derive four types of generating functions of Canonical Transformation and the Maxwell's relations in thermodynamics.

3. Compare three concepts: "physical space", "configuration space" and "phase space".

Lecture Notes 2 Review of Classical Electrodynamics

Contents

- Vector Analysis (Vector Algebra + Vector Calculus);
- Experimental Law and Maxwell's Equations;
- Multipole Expansions;
- Charged Particles in Electromagnetic Field.

3-Dimensional Euclidean space ($\mathbb{R}^3$)

$\boldsymbol{x} = x_1\boldsymbol{e}_1 + x_2\boldsymbol{e}_2 + x_3\boldsymbol{e}_3 = x_i\boldsymbol{e}_i$, $(i = 1, 2, 3)$. (Einstein's convention, i: dummy index, 哑指标)

Inner product of the basis:

$$\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij} = \begin{cases} 1, & \text{(normalized)} \\ 0, & \text{(orthogonal)} \end{cases} \qquad (i, j = 1, 2, 3).$$

where δ_{ij} is called Kronecker tensor, which is a symmetric tensor.

Basics of inner product/cross product

$$\begin{cases} \boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij}, \\ \boldsymbol{e}_i \times \boldsymbol{e}_j = \epsilon_{ijk}\boldsymbol{e}_k, \quad (i, j, k = 1, 2, 3). \end{cases}$$

Two important tensors:

1. Kronecker tensor (symmetric tensor):

$$\delta_{ij} = \delta_{ji}; \quad A_i\delta_{ij} = A_j.$$

2. Levi-Civita symbol (tensor) (anti-symmetric tensor):

$$\epsilon_{ijk} = \begin{cases} +1, & \text{(even permutation)} \\ -1, & \text{(odd permutation)} \\ 0. & \text{(no order)} \end{cases}$$

where

$$\epsilon_{123}=\epsilon_{231}=\epsilon_{312}=1;\quad \epsilon_{213}=\epsilon_{321}=\epsilon_{132}=\cdots=-1,\quad \epsilon_{112}=\cdots=0.$$

Properties of δ_{ij} and ϵ_{ijk}:

For a symmetric tensor F_{ij}, i.e., $F_{ij}=F_{ji}$, one has

$$\epsilon_{ijk}F_{ij}=0.$$

[Proof]

$$\begin{aligned}\epsilon_{ijk}F_{ij}&=\frac{1}{2}\epsilon_{ijk}\left(F_{ij}+F_{ji}\right)\\&=\frac{1}{2}\epsilon_{ijk}F_{ij}-\frac{1}{2}\epsilon_{jik}F_{ji}=\frac{1}{2}\epsilon_{ijk}\left(F_{ij}-F_{ij}\right)=0.\end{aligned}$$

Some important formulae:

(1)

$$\boldsymbol{e_i}\cdot\boldsymbol{e_j}=\delta_{ij}.$$

(2)

$$\boldsymbol{e_i}\times\boldsymbol{e_j}=\epsilon_{ijk}\boldsymbol{e_k}.$$

(3) For $F_{ij}=F_{ji}$, one has

$$\epsilon_{ijk}F_{ij}\equiv 0.$$

(4)

$$\boldsymbol{A}\cdot\boldsymbol{B}=(A_i\boldsymbol{e}_i)\cdot(B_j\boldsymbol{e}_j)=A_iB_j\left(\boldsymbol{e}_i\cdot\boldsymbol{e}_j\right)=A_iB_j\delta_{ij}=A_iB_i.$$

(5)

$$\begin{aligned}\boldsymbol{A}\times\boldsymbol{B}&=(A_i\boldsymbol{e}_i)\times(B_j\boldsymbol{e}_j)=A_iB_j\left(\boldsymbol{e}_i\times\boldsymbol{e}_j\right)=A_iB_j\epsilon_{ijk}\boldsymbol{e}_k\\&=\left(\epsilon_{kij}A_iB_j\right)\boldsymbol{e}_k=(\boldsymbol{A}\times\boldsymbol{B})_k\boldsymbol{e}_k\ \Rightarrow\ (\boldsymbol{A}\times\boldsymbol{B})_k=\epsilon_{kij}A_iB_j.\end{aligned}$$

(6)

$$\epsilon_{ijk}=\boldsymbol{e}_i\cdot(\boldsymbol{e}_j\times\boldsymbol{e}_k)=\begin{vmatrix}\delta_{1i}&\delta_{2i}&\delta_{3i}\\\delta_{1j}&\delta_{2j}&\delta_{3j}\\\delta_{1k}&\delta_{2k}&\delta_{3k}\end{vmatrix}.$$

(7)

$$\boldsymbol{A}\times\boldsymbol{B}=\begin{vmatrix}\boldsymbol{e}_1 & \boldsymbol{e}_2 & \boldsymbol{e}_3\\ A_1 & A_2 & A_3\\ B_1 & B_2 & B_3\end{vmatrix}=\epsilon_{ijk}M_{1i}M_{2j}M_{3k}=\epsilon_{ijk}\boldsymbol{e}_iA_jB_k$$
$$=\left(\epsilon_{ijk}A_jB_k\right)\boldsymbol{e}_i=(\boldsymbol{A}\times\boldsymbol{B})_i\boldsymbol{e}_i.$$

Noting that $\det(M)=\epsilon_{i_1i_2\cdots i_n}M_{1i_1}M_{2i_2}\cdots M_{ni_n}$,

one has

$$\epsilon_{ijk}\epsilon_{lmn}=\begin{vmatrix}\delta_{il} & \delta_{im} & \delta_{in}\\ \delta_{jl} & \delta_{jm} & \delta_{jn}\\ \delta_{kl} & \delta_{km} & \delta_{kn}\end{vmatrix},$$

$$\Longrightarrow\quad \epsilon_{ijk}\epsilon_{klm}=\epsilon_{ijk}\epsilon_{lmk}=\left(\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl}\right).$$

Exercise:

(1)

$$\boldsymbol{A}\cdot(\boldsymbol{B}\times\boldsymbol{C})=\boldsymbol{B}\cdot(\boldsymbol{C}\times\boldsymbol{A})=\boldsymbol{C}\cdot(\boldsymbol{A}\times\boldsymbol{B}).$$

which coincides with the expression of volume of parallelepiped (平行六面体体积):

$$V=|\boldsymbol{A}\cdot(\boldsymbol{B}\times\boldsymbol{C})|=|\boldsymbol{B}\cdot(\boldsymbol{C}\times\boldsymbol{A})|=|\boldsymbol{C}\cdot(\boldsymbol{A}\times\boldsymbol{B})|.$$

In fact,

$$\boldsymbol{A}\cdot(\boldsymbol{B}\times\boldsymbol{C})=A_i(\boldsymbol{B}\times\boldsymbol{C})_i=A_i\epsilon_{ijk}B_jC_k=\epsilon_{jki}B_jC_kA_i=\boldsymbol{B}\cdot(\boldsymbol{C}\times\boldsymbol{A})=\epsilon_{kij}C_kA_iB_j=\boldsymbol{C}\cdot(\boldsymbol{A}\times\boldsymbol{B}).$$

(2)

$$\boldsymbol{\nabla}(uv)=u\boldsymbol{\nabla}v+v\boldsymbol{\nabla}u.$$

(3)

$$\boldsymbol{\nabla}(\boldsymbol{A}\cdot\boldsymbol{B})=\boldsymbol{A}\times(\boldsymbol{\nabla}\times\boldsymbol{B})+(\boldsymbol{A}\cdot\boldsymbol{\nabla})\boldsymbol{B}+\boldsymbol{B}\times(\boldsymbol{\nabla}\cdot\boldsymbol{A})+(\boldsymbol{B}\cdot\boldsymbol{\nabla})\boldsymbol{A}.$$

(4)

$$\boldsymbol{\nabla}\cdot(\boldsymbol{A}\times\boldsymbol{B})=\boldsymbol{B}\cdot(\boldsymbol{\nabla}\times\boldsymbol{A})-\boldsymbol{A}\cdot(\boldsymbol{\nabla}\times\boldsymbol{B}).$$

(5)

$$\boldsymbol{\nabla}\times(\boldsymbol{A}\times\boldsymbol{B})=(\boldsymbol{B}\cdot\boldsymbol{\nabla})\boldsymbol{A}+(\boldsymbol{\nabla}\cdot\boldsymbol{B})\boldsymbol{A}-(\boldsymbol{A}\cdot\boldsymbol{\nabla})\boldsymbol{B}-(\boldsymbol{\nabla}\cdot\boldsymbol{A})\boldsymbol{B}.$$

(6)

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{A})=\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{A})-\boldsymbol{\nabla}^2\boldsymbol{A}.$$

(7)

$$\boldsymbol{\nabla}\times\boldsymbol{\nabla}\phi\equiv 0.$$

(8)

$$\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\boldsymbol{A})\equiv 0.$$

(9)

$$\begin{cases}\boldsymbol{\nabla}^2\left(\dfrac{1}{r}\right)=4\pi\delta^{(3)}(\boldsymbol{x}),\\ \boldsymbol{\nabla}\left(\dfrac{1}{r}\right)=-\dfrac{\boldsymbol{x}}{r^3}.\end{cases}\qquad\left(r=\sqrt{x_1^2+x_2^2+x_3^2},\boldsymbol{x}=x_1\boldsymbol{e}_1+x_2\boldsymbol{e}_2+x_3\boldsymbol{e}_3\right).$$

Generalized Stokes' theorem (Stokes-Cartan's theorem)

$$\int_{\partial\Omega}\omega=\int_{\Omega}\mathrm{d}\omega.$$

Several special cases of Stokes-Cartan's theorem:

Newton-Leibniz theorem (fundamental):

$$\int_a^b\mathrm{d}f=f(b)-f(a).$$

Green's theorem:

$$\oint_c f\mathrm{d}x+g\mathrm{d}y=\iint_D\left(\frac{\partial g}{\partial x}-\frac{\partial f}{\partial y}\right)\mathrm{d}x\mathrm{d}y.$$

Kelvin-Stokes' theorem:

$$\begin{cases}\oint_L\boldsymbol{F}\cdot\mathrm{d}\boldsymbol{l}=\iint_\Sigma(\boldsymbol{\nabla}\times\boldsymbol{F})\cdot\mathrm{d}\boldsymbol{\Sigma};\\ \oint_L\psi\mathrm{d}\boldsymbol{l}=\iint_\Sigma(\hat{\boldsymbol{n}}\times\boldsymbol{\nabla}\psi)\mathrm{d}\Sigma=\iint\mathrm{d}\boldsymbol{\Sigma}\times\boldsymbol{\nabla}\psi.\end{cases}\quad(\hat{\boldsymbol{n}}=\mathrm{d}\boldsymbol{\Sigma}/\mathrm{d}\left|\boldsymbol{\Sigma}\right|).$$

Gauss-Ostrogradsky's theorem:

$$\begin{cases} \oiint_{\Sigma} \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{\Sigma} = \int_{V} (\boldsymbol{\nabla} \cdot \boldsymbol{F}) \mathrm{d}V, \\ \oiint_{\Sigma} \psi \hat{\boldsymbol{n}} \mathrm{d}\Sigma = \oiint_{\Sigma} \psi \mathrm{d}\boldsymbol{\Sigma} = \int_{r} \boldsymbol{\nabla} \psi \mathrm{d}V, \\ \oiint (\hat{\boldsymbol{n}} \times \boldsymbol{A}) \mathrm{d}\Sigma = \oint_{\Sigma} \mathrm{d}\boldsymbol{\Sigma} \times \boldsymbol{A} = \int_{V} (\boldsymbol{\nabla} \times \boldsymbol{A}) \mathrm{d}V. \end{cases}$$

Helmholtz's theorem of decomposition of vectors:

$\forall\ \boldsymbol{F}$ (continuous and differentiable), one has the following decomposition,

$$\boldsymbol{F} = \boldsymbol{F}_{\parallel} + \boldsymbol{F}_{\perp},$$

where

$$\boldsymbol{\nabla} \times \boldsymbol{F}_{\parallel} \equiv 0 \longleftrightarrow \boldsymbol{F}_{\parallel} = -\boldsymbol{\nabla}\phi, \quad \text{(curl-free)}$$
$$\boldsymbol{\nabla} \cdot \boldsymbol{F}_{\perp} = 0 \longleftrightarrow \boldsymbol{F}_{\parallel} = \boldsymbol{\nabla} \times \boldsymbol{A}. \quad \text{(divergence-free)}$$

Experimental Laws (Gauss Units)

1. **Coulomb's law:**

$$\boldsymbol{E}(\boldsymbol{x}) = \int_{V'} \frac{\rho(\boldsymbol{x}')(\boldsymbol{x} - \boldsymbol{x}')}{|\boldsymbol{x} - \boldsymbol{x}'|^3} \mathrm{d}^3\boldsymbol{x}' = -\boldsymbol{\nabla}\phi(\boldsymbol{x});$$

where

$$\phi(\boldsymbol{x}) = \int_{v'} \frac{\rho(\boldsymbol{x}')}{|\boldsymbol{x} - \boldsymbol{x}'|} \mathrm{d}^3\boldsymbol{x}',$$

and after some algebra one yields,

$$\boldsymbol{\nabla} \cdot \boldsymbol{E} \equiv 4\pi\rho(\boldsymbol{x}). \quad \text{(Gauss's law)}.$$

2. **Biot-Savart's law:**

$$\boldsymbol{B}(\boldsymbol{x}) = \int \frac{\boldsymbol{j}(\boldsymbol{x}') \times (\boldsymbol{x} - \boldsymbol{x}')}{|\boldsymbol{x} - \boldsymbol{x}'|} \mathrm{d}^3\boldsymbol{x}' = \boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{x});$$

where

$$\boldsymbol{A}(\boldsymbol{x}) = \int_{\nu} \frac{\boldsymbol{j}(\boldsymbol{x}')}{|\boldsymbol{x} - \boldsymbol{x}'|} \mathrm{d}^3\boldsymbol{x}',$$

and after some algebra one yields,

$$\boldsymbol{\nabla} \cdot \boldsymbol{B} \equiv 0. \quad \text{(Gauss's magnetic law)}.$$

3. Ampere's law (circuit):

$$\oint_L \boldsymbol{B}\cdot \mathrm{d}\boldsymbol{l} = \frac{4\pi}{c}\iint_\Sigma \boldsymbol{j}\cdot \mathrm{d}\boldsymbol{\Sigma},$$

from which, after some algebra, one yields

$$\boldsymbol{\nabla}\times\boldsymbol{B} = \frac{4\pi}{c}\boldsymbol{j}.$$

4. Faraday's law (induction):

$$\oint_L \boldsymbol{E}\cdot \mathrm{d}\boldsymbol{l} = -\frac{1}{c}\int \frac{\partial \boldsymbol{B}}{\partial t}\cdot \mathrm{d}\boldsymbol{\Sigma},$$

from which, after some algebra, one yields

$$\boldsymbol{\nabla}\times\boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{B}}{\partial t}.$$

5. Conservation of electric charge (continuity equation):

$$\left.\begin{array}{l} \dfrac{\mathrm{d}Q}{\mathrm{d}t}\equiv 0, \\ Q=\displaystyle\int_V \rho(\boldsymbol{x})\mathrm{d}^3\boldsymbol{x}. \end{array}\right\} \Longrightarrow \frac{\partial\rho}{\partial t}+\boldsymbol{\nabla}\cdot\boldsymbol{j}\equiv 0.$$

Maxwell's equations

Maxwell's equations:

$$\begin{cases} \boldsymbol{\nabla}\cdot\boldsymbol{E} = 4\pi\rho, \\ \boldsymbol{\nabla}\cdot\boldsymbol{B} = 0, \\ \boldsymbol{\nabla}\times\boldsymbol{B} = \dfrac{4\pi}{c}\boldsymbol{j}+\dfrac{1}{c}\dfrac{\partial\boldsymbol{E}}{\partial t} = \dfrac{4\pi}{c}\left(\boldsymbol{j}+\boldsymbol{j}_{\mathrm{D}}\right), \\ \boldsymbol{\nabla}\times\boldsymbol{E} = -\dfrac{1}{c}\dfrac{\partial\boldsymbol{B}}{\partial t}. \end{cases}$$

Displacement current:

$$\boldsymbol{j}_{\mathrm{D}} = \frac{1}{4\pi}\frac{\partial\boldsymbol{E}}{\partial t}.$$

Lorentz-Newton's equation:

$$\begin{cases} m_a\ddot{\boldsymbol{x}}_a(t) = q_a\left[\boldsymbol{E}\left(\boldsymbol{x}_a(t),t\right)+\dfrac{\boldsymbol{v}_a(t)}{c}\times\boldsymbol{B}\left(\boldsymbol{x}_a(t),t\right)\right], \\ \rho(\boldsymbol{x},t)=\sum_a q_a\delta\left(\boldsymbol{x}-\boldsymbol{x}_a(t)\right), \quad \boldsymbol{j}\left(\boldsymbol{x},t\right)=\sum_a q_a\boldsymbol{v}_a(t)\delta\left(\boldsymbol{x}-\boldsymbol{x}_a(t)\right). \end{cases}$$

Scalar/vector potentials:

$$\begin{cases} \boldsymbol{E} = -\boldsymbol{\nabla}\phi - \dfrac{1}{c}\dfrac{\partial}{\partial t}\boldsymbol{A}, & \text{(longitudinal+transverse)} \\ \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}. & \text{(transverse)} \end{cases}$$

Gauge invariance:

$$\begin{cases} \phi \to \phi' - \dfrac{1}{c}\dfrac{\partial}{\partial t}\chi, \\ \boldsymbol{A} \to \boldsymbol{A}' + \boldsymbol{\nabla}\chi. \end{cases} \Longrightarrow \boldsymbol{E}' = \boldsymbol{E}, \quad \boldsymbol{B}' = \boldsymbol{B}. \quad \text{(keep unchanged)}$$

Coulomb gauge and Lorentz gauge:

$$\boldsymbol{\nabla} \cdot \boldsymbol{A} \equiv 0; \quad \boldsymbol{\nabla} \cdot \boldsymbol{A} + \frac{1}{c}\frac{\partial}{\partial t}\chi \equiv 0.$$

Multipole expansions:

$$\phi = \int_{V'} \frac{\rho\left(\boldsymbol{x}'\right)}{|\boldsymbol{x} - \boldsymbol{x}'|}\mathrm{d}^3\boldsymbol{x}', \quad \boldsymbol{A} = \frac{1}{c}\int \frac{\boldsymbol{j}\left(\boldsymbol{x}'\right)}{|\boldsymbol{x} - \boldsymbol{x}'|}\mathrm{d}^3\boldsymbol{x}'.$$

where $R = \dfrac{1}{|\boldsymbol{x}|}$, $|\boldsymbol{x}'| \ll |\boldsymbol{x}|$

$$\frac{1}{(\boldsymbol{x} - \boldsymbol{x}')} = \frac{1}{R} - \boldsymbol{x} \cdot \boldsymbol{\nabla}\left(\frac{1}{R}\right) + \frac{1}{2!}\left(-\boldsymbol{x}' \cdot \boldsymbol{\nabla}\right)^2\left(\frac{1}{R}\right) + \cdots,$$

$$\Longrightarrow \qquad \phi(\boldsymbol{x}) = \phi^{(0)} + \phi^{(1)} + \phi^{(2)} + \cdots,$$

where $\phi^{(0)} \leftrightarrow$ point charge, $\phi^{(1)} \leftrightarrow$ electric-dipole, $\phi^{(3)} \to$ electric-quadropole.

$$\phi^{(0)} = \frac{Q}{R}, \quad Q = \int_{V'} \rho\left(\boldsymbol{x}'\right)\mathrm{d}^3\boldsymbol{x}';$$

$$\phi^{(1)} = -\boldsymbol{d} \cdot \boldsymbol{\nabla}\left(\frac{1}{R}\right), \quad \boldsymbol{d} = \int_{V'} \boldsymbol{x}'\rho\left(\boldsymbol{x}'\right)\mathrm{d}^3\boldsymbol{x}';$$

$$\Longrightarrow \quad \boldsymbol{E} = -\boldsymbol{\nabla}\phi = \boldsymbol{E}^{(0)} + \boldsymbol{E}^{(1)} + \boldsymbol{E}^{(2)} + \cdots,$$

where $\boldsymbol{E}^{(0)} = \dfrac{Q}{R^3}\boldsymbol{x}$, $\boldsymbol{E}^{(1)} = \dfrac{3\left(\boldsymbol{d} \cdot \hat{\boldsymbol{n}}\right)\hat{\boldsymbol{n}} - \boldsymbol{d}}{R^3}$, $\hat{\boldsymbol{n}} = \dfrac{\boldsymbol{x}}{R}$.

Exterior electric field on charged particles:

$$\begin{aligned} W &= W^{(0)} + W^{(1)} + W^{(2)} + \cdots \\ &= q\phi^{(0)} - \boldsymbol{d}\cdot\boldsymbol{E}(0) - \frac{1}{6}\sum_{ij} Q_{ij}\frac{\partial E_j(0)}{\partial x_i} + \cdots, \end{aligned}$$

$W^{(0)} = q\phi^{(0)}$, electric-monopole (electric charge) interaction

$W^{(1)} = -\boldsymbol{d}\cdot\boldsymbol{E}(0)$, electric-dipole interaction

$W^{(2)} = -\frac{1}{6}\overrightarrow{\overrightarrow{\boldsymbol{Q}}}\cdot\boldsymbol{\nabla}\boldsymbol{E}$. electric-quadropole interaction

For magnetic field

$$\boldsymbol{A}(\boldsymbol{x}) = \boldsymbol{A}^{(0)} + \boldsymbol{A}^{(1)} + \cdots,$$

$$\boldsymbol{A}^{(0)} = \frac{1}{cR}\int_{V'} \boldsymbol{j}\left(\boldsymbol{x}'\right)\mathrm{d}^3\boldsymbol{x}' \equiv 0, \qquad \text{(no monopole)}$$

$$\begin{cases} \boldsymbol{A}^{(1)} = \dfrac{1}{c}\dfrac{\boldsymbol{m}\times\boldsymbol{x}}{R^3}, \\ \boldsymbol{\mu} = \dfrac{1}{2c}\displaystyle\int_{V'} \boldsymbol{x}'\times\boldsymbol{j}\left(\boldsymbol{x}'\right)\mathrm{d}^3x' = \frac{I}{2c}\oint \boldsymbol{x}'\times\mathrm{d}\boldsymbol{l}', \end{cases}$$

$$\Longrightarrow \quad \boldsymbol{B}(\boldsymbol{x}) = \boldsymbol{B}^{(1)}(\boldsymbol{x}) = \boldsymbol{\nabla}\times\boldsymbol{A}^{(1)} = \frac{1}{c}\frac{3(\hat{\boldsymbol{n}}\cdot\boldsymbol{\mu})\hat{\boldsymbol{n}} - \boldsymbol{\mu}}{R^3}, \quad (\boldsymbol{n} = \frac{\boldsymbol{x}}{R}). \text{ (magnetic dipole)}$$

where

$$\begin{aligned} \boldsymbol{j} &= \sum_i q_i\boldsymbol{v}_i\delta\left(\boldsymbol{x}-\boldsymbol{x}_i\right); \\ \boldsymbol{\mu} &= \frac{1}{2c}\int_{V'} \boldsymbol{x}'\times\boldsymbol{j}\left(\boldsymbol{x}'\right)\mathrm{d}^3\boldsymbol{x}' = \frac{1}{2c}\sum_i q_i\left(\boldsymbol{x}_i\times\boldsymbol{v}_i\right) = \sum_i \frac{q_i}{2m_ic}\overrightarrow{L_i}; \\ \boldsymbol{F} &= \int_{V'} \boldsymbol{j}\left(\boldsymbol{x}'\right)\times\boldsymbol{B}\left(\boldsymbol{x}'\right)\mathrm{d}^3\boldsymbol{x}' \\ &= (\boldsymbol{\mu}\times\boldsymbol{\nabla})\times\boldsymbol{B} \\ &= \boldsymbol{\nabla}(\boldsymbol{\mu}\cdot\boldsymbol{B}) - \boldsymbol{\mu}(\boldsymbol{\nabla}\cdot\boldsymbol{B}) = \boldsymbol{\nabla}(\boldsymbol{\mu}\cdot\boldsymbol{B}) = -\boldsymbol{\nabla}U; \\ U &= -\boldsymbol{\mu}\cdot\boldsymbol{B} \\ &= -\sum_i \frac{q_i}{2m_ic}\boldsymbol{L}_i\cdot\boldsymbol{B} \Longrightarrow \quad U = -\frac{q}{2mc}\boldsymbol{L}\cdot\boldsymbol{B}. \quad \text{for single particle.} \end{aligned}$$

Charged particles in electromagnetic field:

Using d'Alembert's principle and generalized force,

$$Q_a = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{q}_a}\right) - \frac{\partial T}{\partial q_a}, \quad (a = 1, 2, \cdots, D),$$

the generalized potential, with $\dot{q}_a$-dependence, can be derived together with the expressions of Lagarangian and Hamiltionian:

$$\begin{cases} L = \frac{1}{2}m\dot{\boldsymbol{x}}^2 - q\phi + \frac{q}{c}\boldsymbol{v}\cdot\boldsymbol{A}, \\ H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}\right)^2 + q\phi. \end{cases}$$

non-holonomic constraint:

$$U(x, \dot{x}; t) \equiv 0,$$

where the canonical momentum (NOT kinetic momentum) is

$$\boldsymbol{p} = m\dot{\boldsymbol{x}} + \frac{q}{c}\boldsymbol{A},$$

or the kinetic momentum is

$$m\dot{\boldsymbol{x}} = \boldsymbol{p} - \frac{q}{c}\boldsymbol{A}.$$

More on Legendre Transformation:

$$f(x) \to g(p) = f(x) - xf'(x) = f(x) - xp \Rightarrow \begin{cases} \frac{\partial g}{\partial x} = f(x) - f(x) \equiv 0, \\ \frac{\partial f}{\partial p} = g' + x \equiv 0. \end{cases}$$

$$f\left(x_i, y_j\right) \to g\left(x_i, p_j\right) = f\left(x_i, y_j\right) - \sum_j y_i \frac{\partial f}{\partial y_i} = f\left(x_i, y_i\right) - \sum_j y_i p_j,$$

$$\Rightarrow 0 \equiv \frac{\partial f}{\partial p_i} = \frac{\partial g}{\partial p_j} + y_j, \ \Rightarrow y_i = -\frac{\partial g}{\partial p_j}; \ \frac{\partial g}{\partial y_i} = \frac{\partial f}{\partial y_j} - \frac{\partial f}{\partial y_j} \equiv 0.$$

Exercises:

1. Prove Helmholtz's theorem.
2. Compare the CGS unit system with the SI unit system.
3. Do all the exercises in Vector analysis.

Lecture Notes 3 Review of Classical Mechanics and Vector Analysis

Contents

- Classical Mechanics and Quantum Mechanics;
- Electrodynamics and Quantum Mechanics;
- Gauge (transformation) Invariance;
- Vector analysis-important formulae. (using Einstein's convention).

Classical Mechanics

Quantum Mechanics $\overset{\text{vs.}}{\longleftrightarrow}$ Classical Mechanics (Canonical Mechanics)

a) Canonical position/momentum (coordinates):

x_i, p_i, $\cdots$ must be canonical.

b) Canonical commutation relation (Poissonian Bracket):

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij} \longleftrightarrow [\hat{x}_i, \hat{p}_j]_{PB} = \delta_{ij},$$
$$\left[\hat{A}, \hat{B}\right] = i\hbar\hat{C} \longleftrightarrow [A, B]_{PB} = C.$$

c) Canonical equation's of motion and its generalization:

$$\left.\begin{array}{l} \textbf{Heisenberg's equation} \\ \dfrac{\mathrm{d}\hat{f}}{\mathrm{d}t} = \dfrac{\partial\hat{f}}{\partial t} + \dfrac{1}{i\hbar}\left[\hat{f}, \hat{H}\right]. \\ \\ \textbf{Ehrenfest's theorem} \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\left\langle\hat{f}\right\rangle = \left\langle\dfrac{\partial\hat{f}}{\partial t}\right\rangle + \dfrac{1}{i\hbar}\left\langle\left[\hat{f}, \hat{H}\right]\right\rangle. \end{array}\right\} \overset{\text{vs.}}{\longleftrightarrow} \frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + [f, H]_{PB}.$$

d) Canonical transformation keeps commutation/equations of motion invariant.

Hamiltonian/Lagrangian:

Regular Lagrangian, and can be chosen to the

$$\det\left|\frac{\partial^2 L}{\partial\dot{q}_i\partial\dot{q}_j}\right|\neq 0\Rightarrow \underbrace{L}_{(q_i,\dot{q}_i)}=\underbrace{T}_{\dot{q}_i-\text{only}}-\underbrace{V}_{q_i-\text{only}}\Rightarrow \underbrace{H}_{(q_i,p_i)}=\underbrace{T}_{\dot{q}_i-\text{only}}+\underbrace{V}_{q_i-\text{only}}.$$

in Quantum Mehcanics, Hamiltonian is chosen so as to

$$\text{Hamiltonian}\leftrightarrow\text{Energy}$$

that

$$H=T+V\leftrightarrow E.$$

More on commutations:

QM		CM
$[\hat{x}_i,\hat{p}_j]=i\hbar\delta_{ij},$	$\xrightarrow{1/i\hbar}$	$[\hat{x}_i,\hat{p}_j]_{PB}=\delta_{ij},$
$[\hat{x}_i,\hat{x}_j]=[\hat{p}_i,\hat{p}_j]\equiv 0.$		$[\hat{x}_i,\hat{x}_j]_{PB}=[\hat{p}_i,\hat{p}_j]_{PB}\equiv 0.$
Fundamental Commutation		Fundamental Commutation
$\Downarrow$		$\Downarrow$
$\left[\hat{L}_i,\hat{L}_j\right]=i\hbar\epsilon_{ijk}\hat{L}_k.$	$\xrightarrow{1/i\hbar}$	$[L_i,L_j]_{PB}=\epsilon_{ijk}L_k.$
$\cdots$		$\cdots$

Canonical conjugate in CM & QM: Dimension analysis

$$\left.\begin{matrix}\text{CM}\\ \text{QM}\end{matrix}\right\}:[qp]=[H\mathrm{d}t]=[L\mathrm{d}t]=\underbrace{[S]}_{\text{Action}}=\underbrace{[\boldsymbol{L}]}_{\text{angular momentum}}.$$

Hamiltonian for charged particles in EM field:

$$\begin{cases}\text{CM:}\quad H=\dfrac{1}{2m}\left(\boldsymbol{p}-\dfrac{q}{c}\boldsymbol{A}\right)^2+q\phi,\begin{cases}\boldsymbol{A}:\text{vector potential}\\ \phi:\text{scalar potential}\end{cases}\\ \text{QM:}\quad \hat{H}=\dfrac{1}{2m}\left(\hat{\boldsymbol{p}}-\dfrac{q}{c}\boldsymbol{A}\right)^2+q\phi.\begin{cases}\boldsymbol{A}:\text{vector potential}\\ \phi:\text{scalar potential}\end{cases}\end{cases}$$

Attention! $\boldsymbol{p}$ here is CANONICAL, NOT KINETIC.

$$\underbrace{\boldsymbol{p}}_{\text{canonical}} = \underbrace{m\boldsymbol{v}}_{\text{kinetic}} + \frac{q}{c}\boldsymbol{A}, \quad m\boldsymbol{v} = \boldsymbol{p} - \frac{q}{c}\boldsymbol{A}.$$

(Kinetic Momentum = Canonical Momentum - $\frac{q}{c}\boldsymbol{A}$).

The momentum that can be quantized **MUST BE CANONICAL!**

Classical Electrodynamics:

Basics of Maxwell's equations and EM field:

Conservation of charge:

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{j} = 0. \quad \text{(continuity equation)}$$

Maxwell-Lorentz's equations:

$$\begin{cases} \underbrace{\boldsymbol{\nabla} \cdot \boldsymbol{E} = 4\pi\rho}_{\substack{\text{transverse+} \\ \text{longitudinal (multipole)}}} \quad , \quad \underbrace{\boldsymbol{\nabla} \cdot \boldsymbol{B} = 0}_{\substack{\text{transverse-only} \\ \text{(no-monopole)}}} ; \quad \text{(Two Gauss' Law/Divergence)} \\ \boldsymbol{\nabla} \times \boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{B}}{\partial t}; \quad \text{(Faraday + Maxwell)} \\ \boldsymbol{\nabla} \times \boldsymbol{B} = \frac{4\pi}{c}\boldsymbol{j} + \frac{1}{c}\frac{\partial \boldsymbol{E}}{\partial t}; \quad \text{(Ampère + Maxwell)} \\ m\ddot{\boldsymbol{x}} = q\left(\boldsymbol{E} + \frac{\boldsymbol{v}}{c} \times \boldsymbol{B}\right). \quad \text{(Lorentz Force)} \end{cases}$$

Dimensions in Gauss Units:

$$\begin{array}{ccccccccccc} [\boldsymbol{E}] & = & [\boldsymbol{P}] & = & [\boldsymbol{D}] & = & [\boldsymbol{B}] & = & [\boldsymbol{H}] & = & [\boldsymbol{M}]; \\ \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\ \text{electric} & & \text{electric} & & \text{electric} & & \text{magnetic} & & \text{magnetic} & & \text{magnetization} \\ \text{field} & & \text{polarization} & & \text{displacement} & & \text{induction} & & \text{field} & & \end{array}$$

$$[\boldsymbol{A}] = [\phi] = \frac{[\boldsymbol{E}]}{[L]}.$$

NO ϵ_0! **NO** μ_0! **ONLY** 4π.

Gauge Transformation and Gauge invariance:

$$\boldsymbol{E} = -\boldsymbol{\nabla}\phi - \frac{1}{c}\frac{\partial}{\partial t}\boldsymbol{A}, \quad \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}.$$

$$\begin{cases} \phi \to \phi^{'} + \boldsymbol{\nabla}\chi, \\ \boldsymbol{A} \to \boldsymbol{A}' - \dfrac{1}{c}\dfrac{\partial}{\partial t}\chi. \end{cases} \Rightarrow \boldsymbol{E}' = \boldsymbol{E}; \quad \boldsymbol{B}' = \boldsymbol{B}. \quad \text{(invariant)}$$

Important gauge:

a) Coulomb gauge: $\boldsymbol{\nabla} \cdot \boldsymbol{A} = 0$. (sometimes also $\phi = 0$, radiation gauge).

b) Lorenz gauge: $\boldsymbol{\nabla} \cdot \boldsymbol{A} + \dfrac{1}{c}\dfrac{\partial}{\partial t}\phi = 0$. (Relativistic, often).

Lorenz gauge $\leftrightarrow$ Lorentz transformation.

Vector calculus in EM field:

$$\begin{cases} \text{electric dipole interaction: } W_e = -\boldsymbol{d} \cdot \boldsymbol{E}, \quad (\boldsymbol{d} = q\boldsymbol{x}) \\ \text{magnetic dipole interaction: } W_m = -\boldsymbol{\mu} \cdot \boldsymbol{B}. \quad (\boldsymbol{\mu} = \dfrac{q\boldsymbol{L}}{2mc}) \end{cases}$$

Vector analysis-Helmholtz's theorem:

$$\boldsymbol{F} = \underbrace{\boldsymbol{F}_\perp}_{\text{transverse}} + \underbrace{\boldsymbol{F}_\parallel}_{\text{longitudinal}}, \begin{cases} \underbrace{\boldsymbol{\nabla} \times \boldsymbol{F}_\parallel = 0}_{\text{curl-free}}, \ \boldsymbol{F}_\parallel = -\boldsymbol{\nabla}\phi; \quad \text{(gradient field)} \\ \underbrace{\boldsymbol{\nabla} \cdot \boldsymbol{F}_\perp = 0}_{\text{divergence free}}, \ \boldsymbol{F}_\perp = \boldsymbol{\nabla} \times \boldsymbol{A}. \quad \text{(curl field)} \end{cases}$$

Vector analysis-important formulae (using Einstein Convention)

Basics:

$$\boldsymbol{A} \cdot \boldsymbol{B} = A_i B_i,$$
$$(\boldsymbol{A} \times \boldsymbol{B})_i = \epsilon_{ijk} A_j B_k.$$
$$\delta_{ij} = \delta_{ji}, \quad F_i \delta_{ij} = F_j.$$
$$\epsilon_{ijk} = -\epsilon_{jik}. \begin{cases} F_{ij} = F_{ji}, \\ \Downarrow \\ \epsilon_{ijk} F_{ij} = 0. \end{cases} \begin{cases} \delta_{ij} : \text{Kronecher}; \\ \epsilon_{ijk} : \text{Levi-Civita}. \end{cases}$$

Important Properties:

$$\epsilon_{kij}\epsilon_{klm} = \epsilon_{ijk}\epsilon_{klm} = \epsilon_{ijk}\epsilon_{lmk} = \epsilon_{ijk}\epsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}.$$

Exercises:

$$\begin{cases} \boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\boldsymbol{A})=0, \\ \boldsymbol{\nabla}\times\boldsymbol{\nabla}\phi=0, \\ \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\boldsymbol{A})=\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{A})-\boldsymbol{\nabla}^2\boldsymbol{A}, \\ \boldsymbol{A}\cdot(\boldsymbol{B}\times\boldsymbol{C})=\boldsymbol{B}\cdot(\boldsymbol{C}\times\boldsymbol{A})=\boldsymbol{C}\cdot(\boldsymbol{A}\times\boldsymbol{B}). \end{cases}$$

Examples: Poissonian Bracket for orbital angular momentum (OAM):

$$L_i=\epsilon_{ijk}x_jp_k=(\boldsymbol{x}\times\boldsymbol{p})_i.$$

[**Proof**]

Basics:

$$\begin{aligned} &[x_i,x_j]_{PB}=[p_i,p_j]_{PB}\equiv 0, \\ &[x_i,p_j]_{PB}=\delta_{ij}, \\ &[A,B]_{PB}=-[B,A]_{PB}, \\ &[A,BC]_{PB}=[A,B]_{PB}C+B[A,C]_{PB}, \\ &[AB,C]_{PB}=[A,C]_{PB}B+A[B,C]_{PB}. \end{aligned}$$

Question:

$$[L_i,L_j]_{PB}=?$$

Solution:

$$\begin{aligned} [L_i,L_j]_{PB}=&[\epsilon_{iab}x_ap_b,\epsilon_{jcd}x_cp_d]_{PB} \\ =&\epsilon_{iab}\epsilon_{jcd}[x_ap_b,x_cp_d]_{PB} \\ =&\epsilon_{iab}\epsilon_{jcd}\left(x_c[x_a,p_d]_{PB}p_b+x_a[p_b,x_c]_{PB}p_d\right) \\ =&\epsilon_{iab}\epsilon_{jcd}(x_cp_b\delta_{ad}-x_ap_d\delta_{bc}) \\ =&\epsilon_{iab}\epsilon_{jca}x_cp_b-\epsilon_{iab}\epsilon_{jbd}x_ap_d \\ =&\epsilon_{bia}\epsilon_{jca}x_cp_b+\epsilon_{iab}\epsilon_{bjd}x_ap_d \\ =&(\delta_{bj}\delta_{ic}-\delta_{bc}\delta_{ij})x_cp_b+(\delta_{ij}\delta_{ad}-\delta_{id}\delta_{aj})x_ap_d \\ =&x_ip_j\underbrace{-x_bp_b\delta_{ij}+x_ap_a\delta_{ij}}_{=0}-x_jp_i \\ =&x_ip_j-x_jp_i. \end{aligned}$$

$$\begin{aligned}\epsilon_{ijk}L_k =&\epsilon_{ijk}(\boldsymbol{x}\times\boldsymbol{p})_k = \epsilon_{ijk}\epsilon_{klm}x_l p_m\\ =&(\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl})x_l p_m = x_i p_j - x_j p_i.\\ \Longrightarrow\qquad & [L_i, L_j]_{PB} = \epsilon_{ijk}L_k.\end{aligned}$$

Exercises:

1. Express the unit of charge and current in terms of other units (M, L, T) in Gaussian units system. Can this be done in SI units system?

2. Derive the expression of the magnetic dipole.

3. Do the exercises in Vector analysis-important formulae.

Lecture Notes 4 Review of Coordinate Transformation

Contents

- Gauge invariance;
- Electrodynamics used in QM;
- Euclidean space and coordinate transformation.

Gauge (transformation) invariace:

$$\begin{cases} \phi \to \phi' = \phi - \dfrac{1}{c}\dfrac{\partial}{\partial t}\chi, \\ \boldsymbol{A} \to \boldsymbol{A'} = \boldsymbol{A} + \boldsymbol{\nabla}\chi. \end{cases}$$

$$\begin{cases} \boldsymbol{E'} = -\boldsymbol{\nabla}\phi' - \dfrac{1}{c}\dfrac{\partial}{\partial t}\boldsymbol{A'} = -\boldsymbol{\nabla}\Big(\phi - \dfrac{1}{c}\dfrac{\partial}{\partial t}\chi\Big) - \dfrac{1}{c}\dfrac{\partial}{\partial t}\Big(\boldsymbol{A} + \boldsymbol{\nabla}\chi\Big) \\ \quad = \Big(-\boldsymbol{\nabla}\phi - \dfrac{1}{c}\dfrac{\partial}{\partial t}\boldsymbol{A}\Big) + \Big(\dfrac{1}{c}\dfrac{\partial}{\partial t}\boldsymbol{\nabla}\chi - \dfrac{1}{c}\dfrac{\partial}{\partial t}\boldsymbol{\nabla}\chi\Big) = \Big(-\boldsymbol{\nabla}\phi - \dfrac{1}{c}\dfrac{\partial}{\partial t}\boldsymbol{A}\Big) = \boldsymbol{E}, \\ \boldsymbol{B'} = \boldsymbol{\nabla} \times \boldsymbol{A'} = \boldsymbol{\nabla} \times \Big(\boldsymbol{A} + \boldsymbol{\nabla}\chi\Big) = \boldsymbol{\nabla} \times \boldsymbol{A} + \boldsymbol{\nabla} \times \boldsymbol{\nabla}\chi = \boldsymbol{\nabla} \times \boldsymbol{A} = \boldsymbol{B}. \end{cases}$$

Electrodynamics used in QM:

1) $\hat{H} = \dfrac{1}{2m}(\boldsymbol{p} - \dfrac{q}{c}\boldsymbol{A})^2 + q\phi$;

   $\boldsymbol{p}$ is canonical momentum, not kinetic momoentum!

2) multipole expansion:
   a)

$W_e = -\boldsymbol{d} \cdot \boldsymbol{E}$;	$\boldsymbol{d} = q\boldsymbol{x}$;	electric-dipole moment
$\updownarrow$	$\updownarrow$	interaction with electric field.
Stark effect	$\boldsymbol{x}-$ dependent	selection rule
	odd-parity	(different parity) allowed.

b)

$W_m = -\boldsymbol{\mu}\cdot\boldsymbol{B}$;	$\boldsymbol{\mu} = \dfrac{q\boldsymbol{L}}{2mc}$;	magnetic-dipole moment
$\updownarrow$	$\updownarrow$	interaction with magnetic field.
Zeeman effect,	$\boldsymbol{L}-$ dependent	selection rule.
Lamor precession $\cdots$	$(\boldsymbol{x}\times\boldsymbol{p})$ even-parity	(same parity) allowed.

Generalized to Quantum Mechanics:

1) $\hat{H} = \dfrac{1}{2m}\left(\hat{\boldsymbol{p}} - \dfrac{q}{c}\boldsymbol{A}(\boldsymbol{x})\right)^2 + q\phi(\hat{\boldsymbol{x}})$.

2) $\hat{H}_{Ie} = -\hat{\boldsymbol{d}}\cdot\boldsymbol{E}(\boldsymbol{x})$; $\hat{\boldsymbol{d}} = q\hat{\boldsymbol{x}}$. electric-dipolemoment operator

3) $\hat{H}_{Im} = -\hat{\boldsymbol{\mu}}_{\boldsymbol{L}}\cdot\boldsymbol{B}(\hat{\boldsymbol{x}})$; $\hat{\boldsymbol{\mu}}_{\boldsymbol{L}} = \dfrac{q\hat{\boldsymbol{L}}}{2mc}$. orbital magetic moment operator $\leftrightarrow \hat{\boldsymbol{L}}$

(typical quantum, $\hat{\boldsymbol{\mu}}_{\boldsymbol{S}} = \dfrac{q\hat{\boldsymbol{S}}}{mc}$. spin (intrinsic) magnetic moment operator $\leftrightarrow \hat{\boldsymbol{S}}$

and relativistic quantum mechanics)

So, the canonical quantization procedure is:
1) $A \to \hat{A}$, i.e.,
observable (c-number) $\to$ observable operator (q-number);
2) CCC $\to$ QCC,
Poissonian Bracket (Classical canonical commutator) $\to$ Commutator (Quantum canonical commutator);

$$[A, B]_{PB} \to \frac{1}{i\hbar}[\hat{A}, \hat{B}],$$

for example: CM (CCC) .

Fundamental relation:

$$\begin{aligned} [x_i, p_j]_{PB} = \delta_{ij}, &\quad \to \quad [\hat{x_i}, \hat{p_j}] = i\hbar\delta_{ij}. \\ [x_i, x_j]_{PB} = [p_i, p_j]_{PB}, &\quad \to \quad [\hat{x_i}, \hat{x_j}] = [\hat{p_i}, \hat{p_j}] = 0. \end{aligned}$$

Angular momentum:

$$[L_i, L_j]_{PB} = \epsilon_{ijk}L_k, \to \quad [\hat{L_i}, \hat{L_j}] = i\hbar\epsilon_{ijk}L_k.$$

or in another form,

$$\hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = i\hbar \hat{\boldsymbol{L}}.$$

Euclidean space, coordinates and coordinate transformation

$$\begin{aligned}
\boldsymbol{v} &= v_x \boldsymbol{e_x} + v_y \boldsymbol{e_y} + v_z \boldsymbol{e_z} \\
&= v_1 \boldsymbol{e}_1 + v_2 \boldsymbol{e}_2 + v_3 \boldsymbol{e_3} \\
&= v_i \boldsymbol{e_i}, \quad (i = 1, 2, 3) \quad \text{(Einstein's convention)}. \\
&\text{where} \quad v_i = \boldsymbol{e_i} \cdot \boldsymbol{v} \quad \text{is the projection in the } i^{\text{th}}\text{-axis.}
\end{aligned}$$

$$\text{orthonormality} \quad \boldsymbol{e_i} \cdot \boldsymbol{e_j} = \delta_{ij} \quad \begin{cases} 1. & (i = j) \quad \text{(normalization)} \\ 0. & (i \neq j) \quad \text{(orthogonality)} \end{cases}$$

$$\text{completeness} \qquad \sum_i \boldsymbol{e_i} \boldsymbol{e_i} = \boldsymbol{e}_1 \boldsymbol{e}_1 + \boldsymbol{e}_2 \boldsymbol{e}_2 + \boldsymbol{e_3} \boldsymbol{e_3} = \mathbb{1}.$$

$$\text{(resolution of identity)} \quad \boldsymbol{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \boldsymbol{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}.$$

$$\longrightarrow \begin{cases} \boldsymbol{e}_1 \boldsymbol{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ \boldsymbol{e}_2 \boldsymbol{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ \boldsymbol{e_3} \boldsymbol{e_3} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \end{cases}$$

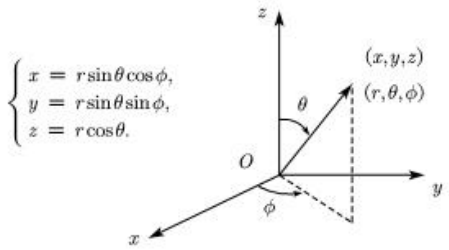
$$\longrightarrow \quad \boldsymbol{e}_1 \boldsymbol{e}_1 + \boldsymbol{e}_2 \boldsymbol{e}_2 + \boldsymbol{e_3} \boldsymbol{e_3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbb{1}_3.$$

Coordinate system

1) rectangular (x, y, z);

2) curvilinear [spherical (r,θ,ϕ)/cyclindrical (ρ,ϕ,z) system].

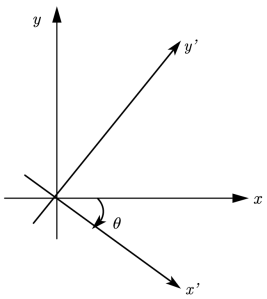
$$\begin{cases} x = r\sin\theta\cos\phi, \\ y = r\sin\theta\sin\phi, \\ z = r\cos\theta. \end{cases}$$



right − hand rule (右手法则)

Some Remarks:

- z-axis: in quantum mechanics, z-axis is defined to be a special axis, termed as "quantum axis". Actually, it is related to the direction of the magnetic field $\boldsymbol{B}$, the direction of which is defined as the quantum axis, denoted by "z" historically.
- Spherical coordinates are adopted in QM in many cases for the simplicity caused by the spherical symmetry in angular momentum (AM)/rotation/atom related topics.
- Spherical coordinate system $\leftrightarrow$ rectangular coordinate system. (mapping well, except two pole points)



Coordinate Transformation (2D case)

$$\begin{aligned} \boldsymbol{v} &= v_x\boldsymbol{e_x} + v_y\boldsymbol{e_y} \\ &= v_i\boldsymbol{e_i} \qquad\qquad (i=1,2) \\ &= v'_j\boldsymbol{e'_j}. \qquad\qquad (j=1,2) \end{aligned}$$

(orthogonal matrix) $\boldsymbol{S}$ (overlapping matrix)

$$\begin{aligned} &\boldsymbol{v} = v_i\boldsymbol{e}_i = v'_j\boldsymbol{e}'_j, \\ &v'_j = (\boldsymbol{e}'_j\cdot\boldsymbol{e_i})v_i = S_{ji}v_i = (\boldsymbol{S})_{ji}v_i. \end{aligned}$$

$$\left.\begin{aligned} v_1' &= (\boldsymbol{e}_1' \cdot \boldsymbol{e}_1)v_1 + (\boldsymbol{e}_1' \cdot \boldsymbol{e}_2)v_2, \\ v_2' &= (\boldsymbol{e}_2' \cdot \boldsymbol{e}_1)v_1 + (\boldsymbol{e}_2' \cdot \boldsymbol{e}_2)v_2. \end{aligned}\right\} \rightarrow \begin{pmatrix} v_1' \\ v_2' \end{pmatrix} = \begin{pmatrix} \boldsymbol{e}_1' \cdot \boldsymbol{e}_1 & \boldsymbol{e}_1' \cdot \boldsymbol{e}_2 \\ \boldsymbol{e}_2' \cdot \boldsymbol{e}_1 & \boldsymbol{e}_2' \cdot \boldsymbol{e}_2 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}.$$

$$\left.\begin{aligned} &\boldsymbol{e}_1' \cdot \boldsymbol{e}_1 = \cos\theta, \boldsymbol{e}_1' \cdot \boldsymbol{e}_2 = \cos(\tfrac{\pi}{2} + \theta) = -\sin\theta, \\ &\boldsymbol{e}_2' \cdot \boldsymbol{e}_1 = \cos(\tfrac{\pi}{2} - \theta) = \sin\theta, \boldsymbol{e}_2' \cdot \boldsymbol{e}_2 = \cos\theta. \end{aligned}\right\} \rightarrow \boldsymbol{S} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

$$\boldsymbol{S}^T = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \rightarrow \boldsymbol{S}^T\boldsymbol{S} = \boldsymbol{S}\boldsymbol{S}^T = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}_2 \rightarrow v' = \boldsymbol{S}v.$$

Actually,

$$v_i = (\boldsymbol{e_i} \cdot \boldsymbol{e_j}')v_j' = (\boldsymbol{S}^{-1})_{ij}v_j' = (\boldsymbol{S}^T)_{ji}v_j',$$

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} \boldsymbol{e}_1 \cdot \boldsymbol{e}_1' & \boldsymbol{e}_1 \cdot \boldsymbol{e}_2' \\ \boldsymbol{e}_2 \cdot \boldsymbol{e}_1' & \boldsymbol{e}_2 \cdot \boldsymbol{e}_2' \end{pmatrix} \begin{pmatrix} v_1' \\ v_2' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} v_1' \\ v_2' \end{pmatrix}, \quad \boldsymbol{v} = \boldsymbol{S}^{-1}\boldsymbol{v'} = \boldsymbol{S}^T\boldsymbol{v'}.$$

Summary of coordinate system

1) $\boldsymbol{S}\boldsymbol{S}^T = \boldsymbol{S}^T\boldsymbol{S} = \mathbb{1}_2$. (orthogonal matrix)
   $\boldsymbol{S}^T = \boldsymbol{S}^{-1}$. (transpose = inverse $\rightarrow$ orthogonal matrix)

2) $\det(\boldsymbol{S}) = \mathbb{1}_2$. (determinant = 1)

3) Transformation of coordinates does NOT change the vector!! (invariant: vector)

4) Coordinate Transformation $\Rightarrow$ Representation Transformation in Quantum Mechanics $\Rightarrow$ Frequently used in Matrix Mechanics and Wave Mechanics in QM.

   Matrix Mechanics: vector (row and column), Observable (matrix);
   Wave Mechanics: vector (wave-fuction), Observable (operator).

Exercises:

1. Compare the dyadic (并矢) with tensor (张量).

2. How to represent an arbitrary rotation in 3D-Euclidean space? Try to give the Coordinate Transformation.

Lecture Notes 5 Fundamental Postulates of QM

Contents

- P.1. State Postulate (S);
- P.2. Operator Postulate (O);
- P.3. Measurement Postulate (M);
- P.4. Evolution Postulate (E);
- P.5. Identical Particle/Symmetrization Postulate (IS).

Fundamental Postulates (Axioms) of QM

P.1 State (Vector) Postulate (S):

$$\text{Physical system} \leftrightarrow \text{State vector} \quad (|\psi\rangle \in \mathbb{H}.\langle\psi| \in \mathbb{H}^*).$$

P.2 Operator Postulate (O):

$$\text{Physical Quantity} \leftrightarrow \text{Observable} \leftrightarrow \text{Operator (Hermitian/Linear)} \quad (\hat{A} : \hat{A}^\dagger = \hat{A}).$$

P.3 Measurement Postulate (M):

1) Measurement Outcomes $\leftrightarrow$ Eigenstate of $\hat{A}$, i.e.,

$$\hat{A}|u_n\rangle = A_n|u_n\rangle.$$

A_n: eigenvalue; $|u_n\rangle$: eigenstate;

2) Probability of measurement outcome A_n:

$$p(A = A_n) = |\langle u_n|\psi\rangle|^2.$$

where

$$|\psi\rangle = \sum_n c_n|u_n\rangle, |c_n|^2 = |\langle u_n|\psi\rangle|^2 \quad (c_n = \langle u_n|\psi\rangle).$$

3) State collapse: $|u_n\rangle$ ($|\psi\rangle \to |u_n\rangle$).

P.4 Evolution Postulate (E):

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle, \quad \text{Schrödinger Equation (SE)},$$

where $\hat{H}$ is the Hamiltonian of the system and can be written as the sum of kinetic energy $\hat{T}$, and potential energy $\hat{V}$, i.e.,

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{\boldsymbol{p}}^2}{2m} + \hat{V}(\boldsymbol{x}).$$

In position-representation, $\hat{\boldsymbol{p}} = -i\hbar\boldsymbol{\nabla} = -i\hbar\dfrac{\partial}{\partial \boldsymbol{x}}$, and SE becomes

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t).$$

SE is a time-dependent partial differential equation, also an initial condition equation, which is determined by the initial condition.

P.5 Identical Particle/Symmetrization Postulate (IS):

Micro-particles are identical particles, which are classified by the spin. The integer-spin particle (boson), is represented by symmetric state vector (wave function); half-integer-spin particles (fermion), is represented by anti-symmetric state vector (wave function).

Discussions

Following discussions are based on P.1-P.3.

P.1 : In Euclidean space, one has

(1) vector addition: commutivity (交换律) $\boldsymbol{v}_1 + \boldsymbol{v}_2 = \boldsymbol{v}_2 + \boldsymbol{v}_1$. $(\forall\ \boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathbb{R}^2)$

(2) scalar multiplication (of a scalar and a vector) (数乘): distributivity (分配律)

$$\begin{cases} a(\boldsymbol{v}_1 + \boldsymbol{v}_2) = a\boldsymbol{v}_1 + a\boldsymbol{v}_2, \\ (a+b)\boldsymbol{v} = a\boldsymbol{v} + b\boldsymbol{v}. \end{cases}$$

(3) inner (dot) product of vectors (内积/标积): commutivity (交换律).

$$r = \boldsymbol{v}_1 \cdot \boldsymbol{v}_2 = \boldsymbol{v}_2 \cdot \boldsymbol{v}_1 = v_{1i} v_{2i}.$$

$$\Longrightarrow \quad v_1^T v_2 = (v_{11} \cdots) \begin{pmatrix} v_{21} \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} = \text{scalar}.$$

(4) Dyadic product of vectors (并矢，外积):

$$v_1 v_2^T = \boldsymbol{v}_1 \boldsymbol{v}_2 \neq \boldsymbol{v}_2 \boldsymbol{v}_1 = \begin{pmatrix} v_{21} \\ v_{22} \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} (v_{11}\ v_{12} \cdots) = \text{matrix}.$$

Basis:

$$\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \underbrace{\delta_{ij}}_{\text{scalar}}, \quad \sum_i \boldsymbol{e}_i \boldsymbol{e}_i = \mathbb{1}_3 = \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{\text{tensor (matrix)}}.$$

In quantum mechanics, the system is depicted as a vector, called state vector (**ket, 右矢**) $|\psi\rangle$ [while **bra (左矢)** $\langle\psi| = (|\psi\rangle)^\dagger$, is its dual (对偶)/conjugate (共轭) $\in \mathbb{H}^*$].

Similar to vectors in Euclidean space, yields:

(1) Vector addition: commutivity (交换律).

$$|\psi_1\rangle + |\psi_2\rangle = |\psi_2\rangle + |\psi_1\rangle.$$

(2) Scalar multiplication: distributivity (分配律).

$$\begin{cases} a\left(|\psi_1\rangle + |\psi_2\rangle\right) = a|\psi_1\rangle + a|\psi_2\rangle, \\ (a_1 + a_2)|\psi\rangle = a_1|\psi\rangle + a_2|\psi\rangle. \end{cases}$$

(3) Inner product of vectors (矢量内积).

$$\langle\psi_1|\psi_2\rangle = (\langle\psi_2|\psi_1\rangle)^* = (\psi_{11}\cdots)\begin{pmatrix}\psi_{21}\\ \cdot\\ \cdot\\ \cdot\end{pmatrix} = \left[(\psi_{21}\cdots)\begin{pmatrix}\psi_{11}\\ \cdot\\ \cdot\\ \cdot\end{pmatrix}\right]^*.$$

(4) Outer (dyadic) product of vectors (矢量外积).

$$\begin{aligned}|\psi\rangle\langle\phi| &= (|\phi\rangle\langle\psi|)^\dagger = (\langle\psi|)^\dagger(|\phi\rangle)^\dagger,\\ |\phi\rangle\langle\psi| &= (\langle\phi|)^\dagger(|\psi\rangle)^\dagger = (|\psi\rangle\langle\phi|)^\dagger.\end{aligned} \quad (\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger.$$

Basis:

1) Discrete basis:

$$\langle u_n|u_m\rangle = \delta_{nm}; \quad \sum_n |u_n\rangle\langle u_n| = \mathbb{1} = \begin{pmatrix}1 & 0 & 0 & \cdots\\ 0 & 1 & 0 & \cdots\\ 0 & 0 & 1 & \cdots\\ \cdots & \cdots & \cdots & \cdots\end{pmatrix}.$$

2) Continuous basis:

$$\langle a|a'\rangle = \delta(a-a'); \quad \int \mathrm{d}a|a\rangle\langle a| = \mathbb{1}.$$

Emphasis:

1) Adjoint $\Big($Hermitian Conjugate (H.C.; h.c.)$\Big)$:

$$(|\psi\rangle)^\dagger = \langle\psi|, \quad (|\psi\rangle\langle\phi|)^\dagger = (\langle\phi|)^\dagger(|\psi\rangle)^\dagger = |\phi\rangle\langle\psi|.$$

2) Inner product:

$$\begin{aligned}&\langle\psi|\phi\rangle = c \in \mathbb{C}, \quad \Big(\langle\psi|\phi\rangle = (\langle\phi|\psi\rangle)^*\Big).\\ &\langle\psi|\psi\rangle = r \in \mathbb{R}, \quad r \geqslant 0, \text{equality iff } |\psi\rangle \equiv \mathbf{0}.\end{aligned}$$

The above are for state vectors (ket/state/$\cdots$).

P.2 : Operator is for operation:

$$\hat{A}|\psi\rangle = |\psi'\rangle.$$

Here are two kinds of operations in QM: $\begin{cases}\text{observable} \leftrightarrow \text{physical quantity.}\\ \text{transformation.}\end{cases}$

(1) Observable Operator: $\hat{H}$ is a *linear Hermitian operator*: $\hat{H}^\dagger = \hat{H}$.

(2) Transformation operators:

Most of the transformation operators are $\begin{cases}\text{linear}\\ \text{unitary}\end{cases}$ operator.

$$\hat{U}^\dagger = \hat{U}^{-1} \text{ or } \hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \mathbb{1}.$$

1. Linearity:

$$\hat{A}(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1\hat{A}|\psi_1\rangle + a_2\hat{A}|\psi_2\rangle. \quad \text{(linearity)}$$

Almost all of the operators are linear in QM (**EXCEPT** Time Reversal operator).

2. Adjoint (hermitian conjugate) (伴随，厄米共轭):

$$\text{Def \#:} \quad \left(\hat{A}|\psi\rangle\right)^\dagger = \langle\psi|\hat{A}^\dagger \Leftrightarrow \langle\phi|\hat{A}^\dagger|\psi\rangle = \left(\langle\psi|\hat{A}|\phi\rangle\right)^*,$$
$$\Longrightarrow \quad \langle\phi|\hat{A}^\dagger|\psi\rangle = \left(\hat{A}|\phi\rangle\right)^\dagger(\langle\psi|)^\dagger = \left[(\langle\psi|)(\hat{A}|\phi\rangle)\right]^\dagger = \left(\langle\psi|\hat{A}|\phi\rangle\right)^\dagger = (\langle\psi|\hat{A}|\phi\rangle)^*.$$

If $\hat{A}$ can be written as a matrix $\Rightarrow \hat{A}^\dagger = \left(\hat{A}^T\right)^* = \left(\tilde{\hat{A}}\right)^*$, transpose + complex conjugate.

$$\left(\hat{A}^\dagger\right)_{ij} = \left(\hat{A}^T\right)^*_{ij} = \left(\hat{A}\right)^*_{ji}.$$

3. Self-adjoint (Hermitian) (自伴，厄米):

If $\hat{A}^\dagger = \hat{A}$, then $\hat{A}$ is a Hermitian (self-adjoint) operator.

$$\Rightarrow \left(\hat{A}^\dagger\right)_{ij} = A^*_{ji} = A_{ij} \Rightarrow \text{hermitian operator } A_{ij} = A^*_{ji}.$$

4. Eigenstate of Hermitian operator:

$$\hat{A}|u_n\rangle = A_n|u_n\rangle. \quad (A_n \in \mathbb{R}). \quad \text{(Discrete)}$$
$$\hat{A}|a\rangle = a|a\rangle. \quad (a \in \mathbb{R}). \quad \text{(Continuous)}$$

Eigenstates/eigenkets/eigenvectors/eigenfunction $\cdots$ constitute an orthonor-

mal and complete basis:

1) DV: $\langle u_n|u_m\rangle = \delta_{nm}$; $\quad \sum_n |u_n\rangle\langle u_n| = \mathbb{1}$.

2) CV: $\langle a|a'\rangle = \delta(a-a')$; $\quad \int \mathrm{d}a|a\rangle\langle a| = \mathbb{1}$.

5. Rules for operators:

What is the meaning of $\hat{A} = \hat{B}$?

$\forall|\psi\rangle$, $\hat{A}|\psi\rangle = \hat{B}|\psi\rangle$.

$\forall|\psi\rangle$, $\left(\hat{A}+\hat{B}\right)|\psi\rangle = \left(\hat{B}+\hat{A}\right)|\psi\rangle = \hat{A}|\psi\rangle + \hat{B}|\psi\rangle$.

1) Commutivity in addition (加法交换律): $\hat{A}+\hat{B} = \hat{B}+\hat{A}$.

2) Associativity in multiplication (乘法结合律): $\left(\hat{A}\hat{B}\right)|\psi\rangle = \hat{A}\left(\hat{B}|\psi\rangle\right)$.

3) Non-commutivity in multiplication (乘法非交换性): $\hat{A}\hat{B} \neq \hat{B}\hat{A}$.

Def # Commutation: $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

4) Associativity in addition (加法结合律): $\left(\hat{A}+\hat{B}\right)+\hat{C} = \hat{A}+\left(\hat{B}+\hat{C}\right)$.

5) Identity (单位算符): $\forall\ |\psi\rangle$, $\hat{A}|\psi\rangle = |\psi\rangle$, then $\hat{A} = \mathbb{1}$.

6) Inverse (逆): $\hat{A}\hat{A}^{-1} = \hat{A}^{-1}\hat{A} = \mathbb{1}$.

$$\left(\hat{A}\hat{B}\right)^{-1} = \hat{B}^{-1}\hat{A}^{-1}, \quad \left(\left(\hat{A}\hat{B}\right)^{-1}\left(\hat{A}\hat{B}\right) = \mathbb{1} = \hat{B}^{-1}\hat{A}^{-1}\hat{A}\hat{B} = \hat{B}^{-1}\hat{B} = \mathbb{1}\right).$$

Definition of inverse:

$$\hat{A}|\psi\rangle = |\phi\rangle \Rightarrow |\psi\rangle = \hat{A}^{-1}|\phi\rangle.$$

7) Function of operators:

$$\begin{cases} f(\hat{A}) = \sum\limits_{n=0}^{\infty} \dfrac{\hat{f}^{(n)}(0)}{n!}\hat{A}^n, \\ f(\hat{A},\hat{B},\cdots) = \sum\limits_{n,m=0}^{\infty} \dfrac{\hat{f}^{n,m,\cdots}(0)}{n!m!\cdots}\hat{A}^n\hat{B}^m\cdots. \end{cases}$$

8) Identities related to commutators:

$$[\hat{A},\hat{B}] = -[\hat{B},\hat{A}].$$
$$[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}].$$
$$\begin{cases} [\hat{A},\hat{B}\hat{C}] = \hat{B}[\hat{A},\hat{C}] + [\hat{A},\hat{B}]\hat{C}, \\ [\hat{A}\hat{B},\hat{C}] = [\hat{A},\hat{C}]\hat{B} + \hat{A}[\hat{B},\hat{C}]. \end{cases} \Rightarrow \begin{array}{l} [\hat{A},\hat{B}^n] = n[\hat{A},\hat{B}]\hat{B}^{n-1}. \\ \Big(\text{condition: } \big[\hat{A},[\hat{A},\hat{B}]\big] = \big[\hat{B},[\hat{A},\hat{B}]\big] \equiv 0\Big) \end{array}$$

Jacobi identity:

$$\big[\hat{A},[\hat{B},\hat{C}]\big] = \big[\hat{B},[\hat{C},\hat{A}]\big] = \big[\hat{C},[\hat{A},\hat{B}]\big] \equiv 0.$$

Remark: Expectation value (mean value) of observables.

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_n |c_n|^2 A_n = \sum_n p(A_n)A_n, \quad \text{(for normalized } |\psi\rangle)$$

or

$$\langle\hat{A}\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle}. \quad \text{(non-normalized } |\psi\rangle).$$

Variance:

$$\sigma_A^2 = \Delta\hat{A}^2 = \left\langle \left(\hat{A} - \langle\hat{A}\rangle\right)^2 \right\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2.$$
$$\sigma_A = \left(\Delta\hat{A}^2\right)^{1/2} = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2}.$$

Exercises:

1. Prove that the commutators satisfy the Jacobi identity.

2. Compare the commutators with Poisson brackets.

Lecture Notes 6 Wave Mechanics and Matrix Mechanics

Contents

- Eigenvalue Problem;
- Schrödinger's Equation and Heisenberg's Equation (Dynamics);
- Matrix Mechanics;
- Wave Mechanics;
- Representation.

Two kinds of problems in QM

1) Eigenvalue equation

$$\begin{cases} \hat{A}|u_n\rangle = A_n|u_n\rangle; & \text{(Discrete eigenspectrum).} \\ \hat{A}|a\rangle = a|a\rangle. & \text{(Continuous eigenspectrum).} \end{cases}$$

2) Evolution equation:

$$\text{Schrödinger's equation: } i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle, \qquad \text{(Schrödinger's Picture)}$$

$$\text{where } |\psi\rangle = |\psi(t)\rangle,\ \frac{\partial\hat{H}}{\partial t} = 0,\ \frac{\mathrm{d}\hat{A}}{\mathrm{d}t} = \frac{\partial\hat{A}}{\partial t} \equiv 0.$$

$$\text{Heisenberg's equation: } \frac{\mathrm{d}\hat{f}}{\mathrm{d}t} = \frac{\partial\hat{f}}{\partial t} + [\hat{f}, \hat{H}], \qquad \text{(Heisenberg's Picture)}$$

$$\text{where } |\psi\rangle = |\psi(0)\rangle \to \frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle \equiv 0.$$

Two kinds of mechanics of QM

1) Matrix Mechanics:

$$\begin{cases} \text{State vector is a row/column vector,} \\ \text{Observable operator is a matrix } (n \times n). \end{cases}$$

2) Wave Mechanics:

$$\begin{cases} \text{State vector is a wavefuction,} \\ \text{Observable operator is an operator in certain representation.} \end{cases}$$

Representation

1) Definition: representation $\leftrightarrow$ basis $\leftrightarrow$ eigenstates of observables $\leftrightarrow$ Linear Hermitian Operator.

2) Eigenstates of Linear Hermitian Operator (Observable).

a)

$$\begin{cases} \text{Discrete basis:} & \hat{A}|u_n\rangle = A_n|u_n\rangle. \\ \text{Continuous basis:} & \hat{A}|a\rangle = a|a\rangle. \\ \text{for example:} & \hat{H}|u_n\rangle = E_n|u_n\rangle;\ \hat{N}|n\rangle = n|n\rangle. \\ & \hat{\boldsymbol{x}}|\boldsymbol{x}\rangle = \boldsymbol{x}|\boldsymbol{x}\rangle;\ \hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle. \end{cases}$$

b) Basis $\leftrightarrow$ orthonormal (orthogonal & normalized) +complete (resolution of identity).

$$\begin{cases} \text{Discrete:} \begin{cases} \langle u_n|u_n\rangle = \delta_{nm} \begin{cases} 0, & (\text{orthogonal},\ n \neq m) \\ 1. & (\text{normalized},\ n = m) \end{cases} \\ \sum\limits_n |u_n\rangle\langle u_n| = \mathbb{1}. \end{cases} \\ \text{Continuous:} \begin{cases} \langle a|a'\rangle = \delta(a - a') \begin{cases} 0, & (\text{orthogonal},\ a \neq a') \\ \infty. & (\text{normalized},\ a = a') \end{cases} \\ \int da|a\rangle\langle a| = \mathbb{1}. \end{cases} \end{cases}$$

c) Theorems of eigenvalues of Hermitian Operators:

$$\hat{H}^\dagger = \hat{H},$$

Hermitian operator (PHY) $\leftrightarrow$ self-adjoint operator (MATH);

Hermitian conjugate = itself (PHY) $\leftrightarrow$ adjoint = itself (MATH).

$$\hat{H}|u_n\rangle = H_n|u_n\rangle. \quad (H_n \in \mathbb{R}).$$

[Proof]:

Let $|u_n\rangle, |u_m\rangle$ are eigenstates of $\hat{H}$, then,

$$\hat{H}|u_n\rangle = H_n|u_n\rangle, \quad \hat{H}|u_m\rangle = H_m|u_m\rangle.$$

According to the definition of Hermitian conjugate, one has

$$\langle u_m|\hat{H}^\dagger|u_n\rangle = (\langle u_n|\hat{H}|u_m\rangle)^* = (\langle u_n|H_m|u_m\rangle)^* = H_m^*\langle u_m|u_n\rangle.$$

Since $\hat{H}^\dagger = \hat{H}$, one yields

$$\langle u_m|\hat{H}|u_n\rangle = \langle u_m|H_n|u_n\rangle = H_n\langle u_m|u_n\rangle.$$

$$\langle u_m|(\hat{H}^\dagger - \hat{H})|u_n\rangle = (H_n - H_m^*)\langle u_m|u_n\rangle = 0 \ \Rightarrow \ \begin{cases} m \neq n, \ \langle u_m|u_n\rangle = 0, \ \text{or} \ |u_m\rangle \perp |u_n\rangle; \\ m = n, \ H_n - H_n^* = 0, \ \text{or} \ H_n \in \mathbb{R}. \end{cases}$$

$$\langle u_n|u_m\rangle = \delta_{nm} \begin{cases} \text{orthogonal.} \\ \text{normalized.} \end{cases}$$

The above proof holds for non-degenerate case, i.e., when $n \neq m$, then $H_n \neq H_m$; for degnerate case, $\hat{H}|u_n^i\rangle = H_n|u_n^i\rangle$, we can use Gram-Schmidt orthonormalization to make: $\langle u_n^i|u_m^i\rangle = \delta_{nm}\delta_{ij}$. (See Advanced Quantum Mechanics Lecture Notes)

Wavefuction and Wave Mechanics

$\hat{\boldsymbol{x}}-, \hat{\boldsymbol{p}}-$ representation. For $\forall$ state vector $|\psi\rangle$, there exists a wave function in a certain representation:

$$\psi(\boldsymbol{x}) = \langle \boldsymbol{x}|\psi\rangle; \quad \psi(\boldsymbol{p}) = \langle \boldsymbol{p}|\psi\rangle.$$

For example, in $\hat{\boldsymbol{x}}-, \hat{\boldsymbol{p}}-$ representation, i.e., adopt the eigenstates of $\boldsymbol{x}$ and $\boldsymbol{p}$, respectively, as the basis, one has:

$$\hat{\boldsymbol{x}}|\boldsymbol{x}\rangle = \boldsymbol{x}|\boldsymbol{x}\rangle; \quad \hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle.$$

$$\begin{cases} \langle \boldsymbol{x}|\boldsymbol{x}'\rangle = \delta(\boldsymbol{x} - \boldsymbol{x}'); \quad \langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p} - \boldsymbol{p}'). \\ \int \mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\langle \boldsymbol{x}| = \mathbb{1}; \quad \int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle \boldsymbol{p}| = \mathbb{1}. \end{cases}$$

For a Hermitian operator $\hat{H}$, i.e.,

$$\hat{H}|\psi\rangle = H_n|\psi\rangle.$$

One has

$$\left.\begin{aligned}\langle \boldsymbol{x}|\hat{H}|\psi\rangle = \langle \boldsymbol{x}|H_n|\psi\rangle = H_n\psi(\boldsymbol{x}),\\ \langle \boldsymbol{x}|\hat{H}|\psi\rangle = \hat{H}\psi(\boldsymbol{x}).\end{aligned}\right\} \to \hat{H}\psi(\boldsymbol{x}) = H_n\psi(\boldsymbol{x}).$$

e.g., Hamiltonian

$$\begin{aligned}\hat{H} =& \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\boldsymbol{x}), \quad \hat{\boldsymbol{p}} = -i\hbar\nabla. \quad (\boldsymbol{x}\text{-representation})\\ \Rightarrow \hat{H}\psi(\boldsymbol{x}) =& -\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x}) + V(\boldsymbol{x})\psi(\boldsymbol{x}).\\ & i\hbar\frac{\partial}{\partial \mathrm{t}}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \Rightarrow i\hbar\frac{\partial}{\partial \mathrm{t}}\psi(\boldsymbol{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x})\right]\psi(\boldsymbol{x},t).\end{aligned}$$

or in $\boldsymbol{p}$-representation:

$$\begin{aligned}&\boldsymbol{x} = i\hbar\nabla_{\boldsymbol{p}}, \quad \hat{H} = \frac{\boldsymbol{p}^2}{2m} + V(i\hbar\nabla_{\boldsymbol{p}}).\\ \Rightarrow \hat{H}\psi(\boldsymbol{p},t) =& \left[\frac{\boldsymbol{p}^2}{2m} + V(i\hbar\nabla_{\boldsymbol{p}})\right]\psi(\boldsymbol{p},t), \quad \psi(\boldsymbol{p},t) = \langle \boldsymbol{p}|\psi(t)\rangle.\end{aligned}$$

Matrix Mechanics: (discret case)

$$\hat{A}|u_n\rangle = A_n|u_n\rangle,$$

$$|\psi\rangle = \mathbb{1}|\psi\rangle = (\sum_n |u_n\rangle\langle u_n|)|\psi\rangle = \sum_n (\langle u_n|\psi\rangle)|u_n\rangle = \sum_n c_n|u_n\rangle = \begin{pmatrix} c_1\\ c_2\\ \vdots\end{pmatrix},$$

$$\langle\psi| = \langle\psi|\mathbb{1} = \langle\psi|(\sum_n |u_n\rangle\langle u_n|) = \sum_n (\langle\psi|u_n\rangle)\langle u_n| = \sum_n c_n^*\langle u_n| = \begin{pmatrix} c_1^* & c_2^* & \cdots\end{pmatrix},$$

$$\begin{aligned}\hat{A} = \mathbb{1}\hat{A}\mathbb{1} &= \sum_{n,m} |u_n\rangle\langle u_n|\hat{A}|u_m\rangle\langle u_m| = \sum_{n,m} (\langle u_n|\hat{A}|u_m\rangle)|u_n\rangle\langle u_m|\\ &= \sum_{n,m} A_{nm}|u_n\rangle\langle u_m| = \begin{pmatrix} A_{11} & \cdots & A_{1m} & \cdots\\ \vdots & & \vdots & \\ A_{n1} & \cdots & A_{nm} & \cdots\\ \vdots & & \vdots & \end{pmatrix}.\end{aligned}$$

where $c_n = \langle u_n|\psi\rangle$, $c_n^* = \langle\psi|u_n\rangle$, $A_{nm} = \langle u_n|\hat{A}|u_m\rangle$.

Adjoint (Hermitian conjugate)

$$\langle\psi|\hat{A}^\dagger|\phi\rangle = (\langle\phi|\hat{A}|\psi\rangle)^*, \begin{cases} |\psi\rangle = \sum_n c_n|u_n\rangle, \\ |\phi\rangle = \sum_n d_n|u_n\rangle. \end{cases}$$

in $\{|u_n\rangle\}$ basis:

$$\begin{aligned} \langle\psi|\hat{A}^\dagger|\phi\rangle &= \langle\psi|(\sum_{n,m}|u_n\rangle\langle u_n|\hat{A}^\dagger|u_m\rangle\langle u_m|)|\phi\rangle \\ &= \sum_{n,m}(\langle u_n|\hat{A}^\dagger|u_m\rangle)c_n^* d_m \\ &= \sum_{n,m}(\hat{A}^\dagger)_{nm}c_n^* d_m. \end{aligned}$$

$$\begin{aligned} (\langle\phi|\hat{A}|\psi\rangle)^* &= \Big(\sum_{n,m}\langle\phi|(|u_m\rangle\langle u_m|)\hat{A}(|u_n\rangle\langle u_n|)|\psi\rangle\Big)^* \\ &= \Big(\sum_{n,m} d_m^* A_{mn} c_n\Big)^* = \sum_{n,m} A_{mn}^* c_n^* d_m; \\ \Longrightarrow \quad & \left(\hat{A}^\dagger\right)_{nm} = A_{mn}^* = \left(A^T\right)_{nm}^* \Rightarrow \hat{A}^\dagger = \left(\hat{A}^T\right)^* = \tilde{\hat{A}}^*. \\ \Longrightarrow \quad & \text{Hermitian conjugate (adjoint) = transpose and complex conjugate.} \end{aligned}$$

$$\hat{A}^\dagger = (\hat{A}^T)^*. \quad (\text{or } \tilde{\hat{A}}^*).$$

For Hermitian operator,

$$\begin{aligned} & \hat{A}^\dagger = \hat{A} \Rightarrow (\hat{A}^T)^* = \hat{A}. \quad \text{(Hermitian operator)} \\ \Longrightarrow \quad & [(\hat{A}^T)^*]_{ij} = A_{ij} = A_{ji}^* \Rightarrow \hat{A}_{ij} = A_{ji}^*. \end{aligned}$$

Exercises:

1. Prove that the eigenvalues of any Hermitian operators must be real.
2. What is your understanding of the "Hermitian conjugate"? (discrete case/continuous case)
3. Prove that $\mathrm{Tr}(\hat{A}\hat{B}\hat{C}) = \mathrm{Tr}(\hat{B}\hat{C}\hat{A}) = \mathrm{Tr}(\hat{C}\hat{A}\hat{B})$, where Tr denotes the trace.
4. Prove that the two definitions of Hermitian Conjugates, i.e., $\langle\psi|\hat{A}^\dagger|\phi\rangle = \Big(\langle\phi|\hat{A}|\psi\rangle\Big)^*$, and $\hat{A}^\dagger|\phi\rangle = \Big(\langle\phi|\hat{A}\Big)^\dagger$ are equivalent.
5. Prove that for degenerate case, the orthonormality of eigenstates also holds.

Lecture Notes 7 Commutations

Contents

- Jacobi Identity;
- Power/Function Related;
- Fundamental Commutations;
- Angular Momentum.

Jacobi Identity:

1. $\left[\hat{A},[\hat{B},\hat{C}]\right]+\left[\hat{B},[\hat{C},\hat{A}]\right]+\left[\hat{C},[\hat{A},\hat{B}]\right]\equiv 0.$

   [**Proof**]

$$\begin{aligned} l.h.s. =& \left[\hat{A}\left(\hat{B}\hat{C}-\hat{C}\hat{B}\right)-\left(\hat{B}\hat{C}-\hat{C}\hat{B}\right)\hat{A}\right]+\left[\hat{B}\left(\hat{C}\hat{A}-\hat{A}\hat{C}\right)-\left(\hat{C}\hat{A}-\hat{A}\hat{C}\right)\hat{B}\right] \\ &+\left[\hat{C}\left(\hat{A}\hat{B}-\hat{B}\hat{A}\right)-\left(\hat{A}\hat{B}-\hat{B}\hat{A}\right)\hat{C}\right] \\ =&\hat{A}\hat{B}\hat{C}-\hat{A}\hat{C}\hat{B}-\hat{B}\hat{C}\hat{A}+\hat{C}\hat{B}\hat{A}+\hat{B}\hat{C}\hat{A}-\hat{B}\hat{A}\hat{C}-\hat{C}\hat{A}\hat{B}+\hat{A}\hat{C}\hat{B}+\hat{C}\hat{A}\hat{B} \\ &-\hat{C}\hat{B}\hat{A}-\hat{A}\hat{B}\hat{C}+\hat{B}\hat{A}\hat{C} \\ \equiv&0. \end{aligned}$$

2. $\boldsymbol{A}\times(\boldsymbol{B}\times\boldsymbol{C})+\boldsymbol{B}\times(\boldsymbol{C}\times\boldsymbol{A})+\boldsymbol{C}\times(\boldsymbol{A}\times\boldsymbol{B})\equiv 0.$

   [**Proof**]

$$\begin{aligned} (l.h.s.)_i =&\epsilon_{ijk}A_j(\boldsymbol{B}\times\boldsymbol{C})_k+\epsilon_{ijk}B_j(\boldsymbol{C}\times\boldsymbol{A})_k+\epsilon_{ijk}C_j(\boldsymbol{A}\times\boldsymbol{B})_k \\ =&\epsilon_{ijk}\epsilon_{klm}\left(A_jB_lC_m+B_jC_lA_m+C_jA_lB_m\right) \\ =&\left(\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl}\right)\left(A_jB_lC_m+B_jC_lA_m+C_jA_lB_m\right) \\ =&A_jB_iC_j+B_jC_iA_j+C_jA_iB_j-A_jB_jC_i-B_jC_jA_i-C_jA_jB_i \\ =&(\boldsymbol{A}\cdot\boldsymbol{C})B_i+(\boldsymbol{A}\cdot\boldsymbol{B})C_i+(\boldsymbol{B}\cdot\boldsymbol{C})A_i-(\boldsymbol{A}\cdot\boldsymbol{B})C_i-(\boldsymbol{B}\cdot\boldsymbol{C})A_i-(\boldsymbol{A}\cdot\boldsymbol{C})B_i \\ \equiv&0. \end{aligned}$$

Leibniz rule:

1. $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$.

   [Proof]

$$\begin{aligned} l.h.s. =& \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A}, \\ r.h.s. =& (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{C} + \hat{B}(\hat{A}\hat{C} - \hat{C}\hat{A}) \\ =& \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A} = l.h.s.. \end{aligned}$$

2. $[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$.

   [Proof]

$$\begin{aligned} l.h.s. =& \hat{A}\hat{B}\hat{C} - \hat{C}\hat{A}\hat{B}, \\ r.h.s. =& (\hat{A}\hat{C} - \hat{C}\hat{A})\hat{B} + \hat{A}(\hat{B}\hat{C} - \hat{C}\hat{B}) \\ =& \hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B} + \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B} = l.h.s.. \end{aligned}$$

Power/Function

1. $\left[\hat{A}, \hat{B}^n\right] = n\left[\hat{A}, \hat{B}\right]\hat{B}^{n-1}$, provided that $\left[\hat{B}, [\hat{A}, \hat{B}]\right] \equiv 0$.

2. $\left[\hat{A}, f(\hat{B})\right] = \left[\hat{A}, \hat{B}\right]\dfrac{\partial f}{\partial \hat{B}}$, provided that $\left[\hat{B}, [\hat{A}, \hat{B}]\right] \equiv 0$.

[Proof]

1. Use MI (mathematical induction, 数学归纳法):

   When $n = 1 \Rightarrow [\hat{A}, \hat{B}] = [\hat{A}, \hat{B}] \Rightarrow$ holds OK.

   $n = 2 \Rightarrow \left[\hat{A}, \hat{B}^2\right] = \hat{B}\left[\hat{A}, \hat{B}\right] + \left[\hat{A}, \hat{B}\right]\hat{B} = 2\left[\hat{A}, \hat{B}\right]\hat{B} \Rightarrow$ holds OK.

   $\cdots$

   Suppose $n = k \Rightarrow \left[\hat{A}, \hat{B}^k\right] = k\left[\hat{A}, \hat{B}\right]\hat{B}^{k-1}$,

   then for $n = k + 1 \Rightarrow$

$$\begin{aligned} \left[\hat{A}, \hat{B}^{k+1}\right] =& \hat{B}\left[\hat{A}, \hat{B}^k\right] + \left[\hat{A}, \hat{B}\right]\hat{B}^k \\ =& \hat{B} \cdot k\left[\hat{A}, \hat{B}\right]\hat{B}^{k-1} + \left[\hat{A}, \hat{B}\right]\hat{B}^k \\ =& k\left[\hat{A}, \hat{B}\right]\hat{B}^k + \left[\hat{A}, \hat{B}\right]\hat{B}^k \\ =& (k+1)\left[\hat{A}, \hat{B}\right]\hat{B}^k. \end{aligned}$$

   Therefore, $\left[\hat{A}, \hat{B}^n\right] = n\left[\hat{A}, \hat{B}\right]\hat{B}^{n-1}$.

2. Do series expansions, we have:

$$
\begin{aligned}
& f(\hat{B})=\sum_n f_n \hat{B}^n, \quad \frac{\partial f}{\partial \hat{B}}=\sum_n n f_n \hat{B}^{n-1}, \\
\Rightarrow & \left[\hat{A}, f(\hat{B})\right]=\left[\hat{A}, \sum_n f_n \hat{B}^n\right]=\sum_n f_n\left[\hat{A}, \hat{B}^n\right]=\sum_n f_n n\left[\hat{A}, \hat{B}\right] \hat{B}^{n-1} \\
= & \left[\hat{A}, \hat{B}\right] \sum_n f_n n \hat{B}^{n-1} \\
= & \left[\hat{A}, \hat{B}\right] \frac{\partial f}{\partial \hat{B}}.
\end{aligned}
$$

Examples: some commutation relations in central potential problems:

Central potential:

$$\hat{V}(\hat{\boldsymbol{x}})=\hat{V}(r).$$

Fundamental commutation:

$$[\hat{x}_i, \hat{p}_j]=i\hbar\delta_{ij}, \quad [\hat{x}_i, \hat{x}_j]=[\hat{p}_i, \hat{p}_j]\equiv 0.$$

So,

a)

$$\left[\hat{p}_i, \hat{V}(r)\right]=[\hat{p}_i, \hat{x}_j]\frac{\partial V}{\partial \hat{x}_j}=-i\hbar\delta_{ij}\cdot\frac{V^{'}}{r}\hat{x}_j=-\frac{i\hbar V^{'}(r)}{r}\hat{x}_i.$$

Note:

$$V=V(r)=V(x_j) \;\Rightarrow\; \frac{\partial V}{\partial x_j}=\frac{\mathrm{d}V}{\mathrm{d}r}\frac{\partial r}{\partial x_j}=\frac{V^{'}}{r}\hat{x}_j.$$

Since

$$[\hat{p}_i, \hat{x}_j]=-i\hbar\delta_{ij}, \quad \left[\hat{x}_k, [\hat{p}_i, \hat{x}_j]\right]\equiv 0,$$

and

$$\hat{L}_i=(\boldsymbol{x}\times\boldsymbol{p})_i=\epsilon_{ijk}\hat{x}_j\hat{p}_k,$$

hence,

$$\left[\hat{L}_i, \hat{x}_j\right]=\epsilon_{ilm}\hat{x}_l\,[\hat{p}_m, \hat{x}_j]=\epsilon_{ilm}\hat{x}_l(-i\hbar\delta_{jm})=\epsilon_{ilj}\hat{x}_l(-i\hbar)=i\hbar\epsilon_{ijk}\hat{x}_k.$$

b)

$$\left[\hat{L}_i, \hat{V}(r)\right] = \left[\hat{L}_i, \hat{x}_j\right] \frac{\partial \hat{V}}{\partial \hat{x}_j} = i\hbar\epsilon_{ijk}\hat{x}_k \cdot \frac{V'}{r}\hat{x}_j = \frac{i\hbar V'}{r}\epsilon_{ijk}\hat{x}_k\hat{x}_j \equiv 0.$$

(symmetric and anti-symmetric tensor).

Fundamental Commutation Relations:

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}; \quad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] \equiv 0.$$

for simplicity, consider $[\hat{x}, \hat{p}_x]$:

Commutation relations do not change in different representations:

(1) in x-representation:

$$\hat{x} = x, \quad \hat{p}_x = -i\hbar\frac{\partial}{\partial x}.$$

$$\Longrightarrow \quad \begin{cases} \psi_p(x) = Ne^{ipx/\hbar}, \\ -i\hbar\psi_p(x) = (-i\hbar)\left(\dfrac{i}{\hbar}p\right) \cdot Ne^{ipx/\hbar} = p\psi_p(x). \end{cases}$$

For $\forall\ \psi(x) = \langle x|\psi\rangle$, one has

$$\begin{aligned} (\hat{x}\hat{p} - \hat{p}\hat{x})\,\psi(x) &= -i\hbar\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right)\psi(x) \\ &= -i\hbar\left[x\frac{\partial}{\partial x}\psi(x) - x\frac{\partial}{\partial x}\psi(x) - \psi(x)\right] \\ &= i\hbar\psi(x) \Rightarrow \hat{x}\hat{p} - \hat{p}\hat{x} = [\hat{x}, \hat{p}_x] = i\hbar. \end{aligned}$$

Similarly,

$$[\hat{y}, \hat{p}_y] = [\hat{z}, \hat{p}_z] = i\hbar.$$

Hence,

$$[\hat{x}_i, \hat{p}_j] = i\hbar, \quad (i = j).$$

And

$$[\hat{x}, \hat{p}_y] = [\hat{x}, \hat{p}_z] = [\hat{y}, \hat{p}_x] = [\hat{y}, \hat{p}_z] = [\hat{z}, \hat{p}_x] = [\hat{z}, \hat{p}_y] \equiv 0.$$

Hence,

$$[\hat{x}_i, \hat{p}_j] = 0, \quad (i \neq j).$$

That is,

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}.$$

We can analogously prove that

$$[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] \equiv 0.$$

(2) in p-representation:

$$\begin{cases} \hat{p} = \hat{p}, \quad \hat{x} = i\hbar \dfrac{\partial}{\partial p}. \\ \psi_x(p) = \psi_p^*(x) = N e^{-ipx/\hbar}. \\ i\hbar \dfrac{\partial}{\partial p} \psi_x(p) = (i\hbar) \dfrac{(-ix)}{\hbar} N e^{-ipx/\hbar} = x\psi_x(p). \end{cases}$$

For $\forall\ \psi(p) \equiv \langle p|\psi\rangle$, one has

$$\begin{aligned} (\hat{x}\hat{p} - \hat{p}\hat{x})\,\psi(p) &= i\hbar \left(\frac{\partial}{\partial p} p - p \frac{\partial}{\partial p} \right) \psi(p) \\ &= i\hbar \left[1 + p\frac{\partial}{\partial p} - p\frac{\partial}{\partial p} \right] \psi(p) \\ &= i\hbar\psi(p) \Rightarrow [\hat{x}, \hat{p}] = i\hbar. \end{aligned}$$

Generally, one has

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}, \quad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] \equiv 0.$$

Angular Momentum (Orbital)

$$\hat{\boldsymbol{L}} = \hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}} \Rightarrow \hat{L}_i = \epsilon_{ijk} \hat{x}_j \hat{p}_k.$$

Commutation Relations:

$$\begin{cases} \left[\hat{L}_i, \hat{x}_j\right] = i\hbar\epsilon_{ijk}\hat{x}_k, \\ \left[\hat{L}_i, \hat{p}_j\right] = i\hbar\epsilon_{ijk}\hat{p}_k, \\ \left[\hat{\boldsymbol{L}}^2, \hat{L}_i\right] \equiv 0. \end{cases} \qquad \begin{cases} \left[\hat{L}_i, \hat{V}(r)\right] \equiv 0, \\ \left[\hat{\boldsymbol{L}}^2, \hat{V}(r)\right] \equiv 0, \\ \left[\hat{L}_z, \hat{V}(r)\right] \equiv 0. \end{cases} \qquad \left[\hat{L}_i, \hat{T}\right] \equiv 0.$$

1. $\left[\hat{L}_i, \hat{L}_j\right] = i\hbar\epsilon_{ijk}\hat{L}_k, \quad \Longleftrightarrow \quad \hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = i\hbar\hat{\boldsymbol{L}}.$

[**Proof**]

$$\begin{aligned}
&\left[\hat{L}_i, \hat{L}_j\right] = \left[\epsilon_{iab}\hat{x}_a\hat{p}_b, \epsilon_{jcd}\hat{x}_c\hat{p}_d\right] \\
&= \epsilon_{iab}\epsilon_{jcd}\Big(\hat{x}_c\left[\hat{x}_a, \hat{p}_d\right]\hat{p}_b + \hat{x}_a\left[\hat{p}_b, \hat{x}_c\right]\hat{p}_d\Big) \\
&= \epsilon_{iab}\epsilon_{jcd}\Big(i\hbar\hat{x}_c\hat{p}_b\delta_{ad} - i\hbar\hat{x}_a\hat{p}_d\delta_{bc}\Big) \\
&= i\hbar\Big(\epsilon_{iab}\epsilon_{jca}\hat{x}_c\hat{p}_b - \epsilon_{ia_b}\epsilon_{jbd}\hat{x}_a\hat{p}_d\Big) \\
&= i\hbar\left(\epsilon_{bi\underline{a}}\epsilon_{jc\underline{a}}\hat{x}_c\hat{p}_b + \epsilon_{ia\underline{b}}\epsilon_{jd\underline{b}}\hat{x}_a\hat{p}_d\right) \\
&= i\hbar\left[\left(\delta_{b_j}\delta_{ic} - \delta_{bc}\delta_{ij}\right)\hat{x}_c\hat{p}_b + \left(\delta_{ij}\delta_{ad} - \delta_{id}\delta_{aj}\right)\hat{x}_a\hat{p}_d\right] \\
&= i\hbar\left[\hat{x}_i\hat{p}_j - (\boldsymbol{x}\cdot\boldsymbol{p})\delta_{ij} + (\boldsymbol{x}\cdot\boldsymbol{p})\delta_{ij} - \hat{x}_j\hat{p}_i\right] \\
&= i\hbar\left(\hat{x}_i\hat{p}_j - \hat{x}_j\hat{p}_i\right).
\end{aligned}$$

On the other hand,

$$\epsilon_{ijk}\hat{L}_k = \epsilon_{ij\underline{k}}\epsilon_{\underline{k}ab}\hat{x}_a\hat{p}_b = \left(\delta_{ia}\delta_{jb} - \delta_{ib}\delta_{ja}\right)\hat{x}_a\hat{p}_b = \hat{x}_i\hat{p}_j - \hat{x}_j\hat{p}_i.$$

Hence,

$$\left[\hat{L}_i, \hat{L}_j\right] = i\hbar\epsilon_{ijk}\hat{L}_k.$$

2. From $\left[\hat{L}_i, \hat{L}_j\right] = i\hbar\epsilon_{ijk}\hat{L}_k \Rightarrow \hat{\boldsymbol{L}}\times\hat{\boldsymbol{L}} = i\hbar\hat{\boldsymbol{L}}$.

[**Proof**]

$$\left.\begin{aligned}
(\hat{\boldsymbol{L}}\times\hat{\boldsymbol{L}})_i &= \epsilon_{ijk}\hat{L}_j\hat{L}_k = \frac{1}{2}\epsilon_{ijk}\hat{L}_j\hat{L}_k + \frac{1}{2}\epsilon_{ijk}\hat{L}_j\hat{L}_k \\
&= \frac{1}{2}\epsilon_{ijk}\hat{L}_j\hat{L}_k - \frac{1}{2}\epsilon_{ikj}\hat{L}_j\hat{L}_k = \frac{1}{2}\epsilon_{ijk}\hat{L}_j\hat{L}_k - \frac{1}{2}\epsilon_{ijk}\hat{L}_k\hat{L}_j \\
&= \frac{1}{2}\epsilon_{ijk}\left(\hat{L}_j\hat{L}_k - \hat{L}_k\hat{L}_j\right) = \frac{1}{2}\epsilon_{ijk}\left[\hat{L}_j, \hat{L}_k\right] \\
&= \frac{1}{2}\epsilon_{ijk}(i\hbar)\epsilon_{jkl}\hat{L}_k = \frac{i\hbar}{2}\epsilon_{ij\underline{k}}\epsilon_{\underline{k}lj}\hat{L}_k \\
&= \frac{i\hbar}{2}\left(\delta_{il}\delta_{jj} - \delta_{ij}\delta_{jl}\right)\hat{L}_k = \frac{i\hbar}{2}\left(3\delta_{il} - \delta_{il}\right)\hat{L}_l \\
&= \frac{i\hbar}{2}\cdot 2\delta_{il}\hat{L}_l = i\hbar\hat{L}_i.
\end{aligned}\right\} \Rightarrow \quad \hat{\boldsymbol{L}}\times\hat{\boldsymbol{L}} = i\hbar\hat{\boldsymbol{L}}.$$

3. From $\hat{\boldsymbol{L}}\times\hat{\boldsymbol{L}} = i\hbar\hat{\boldsymbol{L}} \Rightarrow \left[\hat{L}_i, \hat{L}_j\right] = i\hbar\epsilon_{ijk}\hat{L}_k$.

[**Proof**]

$$\left[\hat{L}_i, \hat{L}_j\right] = i\hbar\epsilon_{ijk}\hat{L}_k,$$

$$\left.\begin{aligned}(\hat{\boldsymbol{L}}\times\hat{\boldsymbol{L}})_i =&\epsilon_{ijk}\hat{L}_j\hat{L}_k = i\hbar\hat{L}_i\\ \Longrightarrow\quad &\epsilon_{ab\underline{i}}\epsilon_{\underline{i}jk}\hat{L}_j\hat{L}_k = i\hbar\epsilon_{abi}\hat{L}_i.\\ \text{where } l.h.s. =&\left(\delta_{aj}\delta_{bk}-\delta_{ak}\delta_{bj}\right)\hat{L}_j\hat{L}_k\\ =&\hat{L}_a\hat{L}_b-\hat{L}_b\hat{L}_a=\left[\hat{L}_a,\hat{L}_b\right].\end{aligned}\right\}\Rightarrow\begin{aligned}&\left[\hat{L}_a,\hat{L}_b\right]=i\hbar\epsilon_{abi}\hat{L}_i\\ &\text{i.e. },\left[\hat{L}_i,\hat{L}_j\right]=i\hbar\epsilon_{ijk}\hat{L}_k.\end{aligned}$$

4. $[\hat{L}_i,\hat{x}_j]=i\hbar\epsilon_{ijk}\hat{x}_k$.

[Proof]

$$\begin{aligned}\left[\hat{L}_i,\hat{x}_j\right]=&\epsilon_{iab}\hat{x}_a\left[\hat{p}_b,\hat{x}_j\right]=-i\hbar\delta_{bj}\epsilon_{iab}\hat{x}_a\\ =&-i\hbar\epsilon_{iaj}\hat{x}_a=i\hbar\epsilon_{ija}\hat{x}_a=i\hbar\epsilon_{ijk}\hat{x}_k.\end{aligned}$$

5. $[\hat{L}_i,\hat{p}_j]=i\hbar\epsilon_{ijk}\hat{p}_k$.

[Proof]

$$\left[\hat{L}_i,\hat{p}_j\right]=\epsilon_{iab}\left[\hat{x}_a,\hat{p}_j\right]\hat{p}_b=\epsilon_{iab}(i\hbar\delta_{aj})\hat{p}_b=i\hbar\epsilon_{ijb}\hat{p}_b=i\hbar\epsilon_{ijk}\hat{p}_k.$$

6. $[\hat{L}_i,\hat{V}(r)]=0$.

[Proof]

$$\begin{aligned}\left[\hat{L}_i,\hat{V}(r)\right]=&\left[\hat{L}_i,\hat{x}_j\right]\frac{\partial\hat{V}}{\partial x_j}=i\hbar\epsilon_{ijk}\hat{x}_k\cdot\frac{\mathrm{d}V}{\mathrm{d}r}\frac{\partial r}{\partial x_j}\\ =&\frac{i\hbar}{r}\left(\frac{\mathrm{d}V}{\mathrm{d}r}\right)\cdot\underbrace{\epsilon_{ijk}}_{\text{anti-symmetric}}\cdot\underbrace{\hat{x}_k\hat{x}_j}_{\text{symmetric}}\equiv 0.\end{aligned}$$

Further, one yields

$$\left[\hat{\boldsymbol{L}}^2,\hat{V}(r)\right]=\hat{L}_i\left[\hat{L}_i,\hat{V}(r)\right]+\left[\hat{L}_i,\hat{V}(r)\right]\hat{L}_i\equiv 0.$$

7. $[\hat{\boldsymbol{L}}^2,\hat{L}_i]=0$.

[Proof]

$$\begin{aligned}&\left[\hat{L}_j\hat{L}_j,\hat{L}_i\right]=\hat{L}_j\left[\hat{L}_j,\hat{L}_i\right]+\left[\hat{L}_j,\hat{L}_i\right]\hat{L}_j\\ &=i\hbar\left[\epsilon_{jik}\hat{L}_j\hat{L}_k+\epsilon_{jik}\hat{L}_k\hat{L}_j\right]\\ &=i\hbar\underbrace{\epsilon_{jik}}_{\text{anti-symmetric}}\underbrace{\left(\hat{L}_j\hat{L}_k+\hat{L}_k\hat{L}_j\right)}_{\text{symmetric}}\\ &\Rightarrow\left[\hat{\boldsymbol{L}}^2,\hat{L}_i\right]\equiv 0.\end{aligned}$$

8. $[\hat{L}_i, \hat{T}] = 0$.

   [Proof]

$$\left[\hat{L}_i, \hat{T}\right] = \left[\hat{L}_i, \frac{\hat{\boldsymbol{p}}^2}{2m}\right] = \left[\hat{L}_i, \hat{p}_j\right]\frac{\hat{p}_j}{2m} + \frac{\hat{p}_j}{2m}\left[\hat{L}_i, \hat{p}_j\right]$$
$$= \frac{1}{2m}\epsilon_{ijk}\left(\hat{p}_k\hat{p}_j + \hat{p}_j\hat{p}_k\right) \equiv 0.$$

Exercises:

1. Prove: $\epsilon_{ijk}\epsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$.
2. From $[\hat{L}_i, \hat{x}_j] = i\hbar\epsilon_{ijk}\hat{x}_k$, derive the expression of $\hat{\boldsymbol{L}} \times \hat{\boldsymbol{x}} + \hat{\boldsymbol{x}} \times \hat{\boldsymbol{L}}$.
3. From $[\hat{L}_i, \hat{p}_j] = i\hbar\epsilon_{ijk}\hat{p}_k$, derive the expression of $\hat{\boldsymbol{L}} \times \hat{\boldsymbol{p}} + \hat{\boldsymbol{p}} \times \hat{\boldsymbol{L}}$.
4. Prove Jacobi identity for commutators and cross products.
5. Prove that $[\hat{A}, f(\hat{B})] = [\hat{A}, \hat{B}]\dfrac{\partial f}{\partial \hat{B}}$ if $\left[\hat{B}, [\hat{A}, \hat{B}]\right] = 0$.
6. Prove all the commutation relations in this lecture.

Lecture Notes 8 Eigenvalue and Eignestate

Contents

- Eigenstates of $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{x}}$ in different representations;
- Eigenstates of angular momentum;
- Ladder operators.

Position in $\boldsymbol{x}$-representation

$$\begin{cases} \hat{\boldsymbol{x}}|\boldsymbol{x}'\rangle = \boldsymbol{x}'|\boldsymbol{x}'\rangle, \\ \int \mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\langle\boldsymbol{x}| = \mathbb{1}. \quad \text{left multiply from both sides.} \end{cases}$$

$$\int \mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\Big(\hat{\boldsymbol{x}}|\boldsymbol{x}'\rangle\Big) = \int \mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\boldsymbol{x}'\langle\boldsymbol{x}|\boldsymbol{x}'\rangle \quad \longrightarrow \quad \langle\boldsymbol{x}|\hat{\boldsymbol{x}}|\boldsymbol{x}'\rangle = \boldsymbol{x}'\delta(\boldsymbol{x}-\boldsymbol{x}').$$

$\langle\boldsymbol{x}|\boldsymbol{x}'\rangle = \delta(\boldsymbol{x}-\boldsymbol{x}')$, wave function of $|\boldsymbol{x}\rangle$ in $\boldsymbol{x}$-representation,
$\hat{\boldsymbol{x}}\delta(\boldsymbol{x}-\boldsymbol{x}') = \boldsymbol{x}'\delta(\boldsymbol{x}-\boldsymbol{x}')$. position operator in $\boldsymbol{x}$-representation.

Momentum in $\boldsymbol{p}$-representation

$$\begin{cases} \hat{\boldsymbol{p}}|\boldsymbol{p}'\rangle = \boldsymbol{p}'|\boldsymbol{p}'\rangle; \\ \int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \mathbb{1}. \quad \text{left multiply from both sides.} \end{cases}$$

$$\int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\Big(\hat{\boldsymbol{p}}|\boldsymbol{p}'\rangle\Big) = \int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\boldsymbol{p}'|\boldsymbol{p}'\rangle \quad \longrightarrow \quad \langle\boldsymbol{p}|\hat{\boldsymbol{p}}|\boldsymbol{p}'\rangle = \boldsymbol{p}'\delta(\boldsymbol{p}-\boldsymbol{p}').$$

$\langle\boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}')$, wave function of $|\boldsymbol{p}\rangle$ in $\boldsymbol{p}$-representation,
$\hat{\boldsymbol{p}}\delta(\boldsymbol{p}-\boldsymbol{p}') = \boldsymbol{p}'\delta(\boldsymbol{p}-\boldsymbol{p}')$. momentum operator in $\boldsymbol{p}$-representation.

Momentum in $\boldsymbol{x}$-representation

$$\hat{\boldsymbol{p}} = -i\hbar\frac{\partial}{\partial\boldsymbol{x}} = -i\hbar\nabla \begin{cases} \int \mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\langle\boldsymbol{x}| = \mathbb{1}, \\ \int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \mathbb{1}. \end{cases}$$

$$|\boldsymbol{p}\rangle = \int \mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\boldsymbol{p}\rangle = \int \mathrm{d}\boldsymbol{x}\Big(\langle\boldsymbol{x}|\boldsymbol{p}\rangle\Big)|\boldsymbol{x}\rangle = \int \mathrm{d}\boldsymbol{x}\psi_{\boldsymbol{p}}(\boldsymbol{x})|\boldsymbol{x}\rangle.$$

$$\left.\begin{aligned}\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle &= \hat{\boldsymbol{p}}\int \mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\boldsymbol{p}\rangle = \int \mathrm{d}\boldsymbol{x}\hat{\boldsymbol{p}}\psi_{\boldsymbol{p}}(\boldsymbol{x})|\boldsymbol{x}\rangle \\ &= \boldsymbol{p}\int \mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\boldsymbol{p}\rangle = \int \mathrm{d}\boldsymbol{x}(-i\hbar\nabla)\psi_{\boldsymbol{p}}(\boldsymbol{x})|\boldsymbol{x}\rangle.\end{aligned}\right\} \longrightarrow \psi_{\boldsymbol{p}}(\boldsymbol{x}) = Ne^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}.$$

$$\mathbb{1} = \int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \int \mathrm{d}\boldsymbol{p}\mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\boldsymbol{x}'\rangle\langle\boldsymbol{x}'|\mathrm{d}\boldsymbol{x}'.$$

$$\begin{aligned}&N^2\int e^{i\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{x}')/\hbar}\mathrm{d}\boldsymbol{p}\int|\boldsymbol{x}\rangle\langle\boldsymbol{x}'|\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{x}' \quad \leftarrow \quad \int e^{ikx}\mathrm{d}k = 2\pi\delta(x), \\ =&N^2\int(2\pi\hbar)^3\delta(\boldsymbol{x}-\boldsymbol{x}')|\boldsymbol{x}\rangle\langle\boldsymbol{x}'|\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{x}' = N^2(2\pi\hbar)^3\int|\boldsymbol{x}\rangle\langle\boldsymbol{x}|\mathrm{d}\boldsymbol{x} = N^2(2\pi\hbar)^3\cdot\mathbb{1} = \mathbb{1}.\end{aligned}$$

$$\Rightarrow \quad N^2\cdot(2\pi\hbar)^3 = 1 \quad \Rightarrow \quad N = \Big(\frac{1}{2\pi\hbar}\Big)^{3/2}.$$

$$\Rightarrow \quad \psi_{\boldsymbol{p}}(\boldsymbol{x}) = \Big(\frac{1}{2\pi\hbar}\Big)^{3/2}e^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} = \langle\boldsymbol{x}|\boldsymbol{p}\rangle.$$

This is the wavefunction of eigenstates of $\hat{\boldsymbol{p}}$ in $\boldsymbol{x}$-representation

$$\Rightarrow \text{ From } \hat{\boldsymbol{p}} = -i\hbar\frac{\partial}{\partial\boldsymbol{x}} \quad \Rightarrow \quad \psi_{\boldsymbol{p}}(\boldsymbol{x}) = \Big(\frac{1}{2\pi\hbar}\Big)^{3/2}e^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}.$$

Similarly, in $\boldsymbol{p}$-represntation,

$$\hat{\boldsymbol{x}} = i\hbar\frac{\partial}{\partial\boldsymbol{p}} \quad \Rightarrow \quad \psi_{\boldsymbol{x}}(\boldsymbol{p}) = \Big(\frac{1}{2\pi\hbar}\Big)^{3/2}e^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}.$$

Furthermore, we can derive the Fundamental Commutation Relation:

$$[\hat{x}_i,\hat{p}_j] = [\hat{x}_i,-i\hbar\frac{\partial}{\partial\hat{x}_j}] = i\hbar\delta_{ij}, \quad [\hat{x}_i,\hat{x}_j] = [\hat{p}_i,\hat{p}_j] \equiv 0.$$

e.g., $\forall\ \psi(x)$

$$\begin{aligned}(\hat{x}\hat{p}_x - \hat{p}_x\hat{x})\psi(x) =& \Big[x\Big(-i\hbar\frac{\partial}{\partial x}\Big) - \Big(-i\hbar\frac{\partial}{\partial x}\Big)x\Big]\psi(x)\\ =& i\hbar\Big[\frac{\partial}{\partial x}\Big(x\psi(x)\Big) - x\frac{\partial}{\partial x}\psi(x)\Big]\\ =& i\hbar\psi(x).\\ \Rightarrow& [\hat{x},\hat{p}_x] = i\hbar,\\ \Rightarrow& [\hat{x}_i,\hat{p}_j] = i\hbar\delta_{ij}.\end{aligned}$$

Summary:

1. In x-representation:

$$\begin{aligned}&\hat{\boldsymbol{x}}|\boldsymbol{x}\rangle = \boldsymbol{x}|\boldsymbol{x}\rangle, \quad \hat{\boldsymbol{x}}\delta(\boldsymbol{x}-\boldsymbol{x}') = \boldsymbol{x}'\delta(\boldsymbol{x}-\boldsymbol{x}').\\ &\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle, \quad \Big(-i\hbar\frac{\partial}{\partial \boldsymbol{x}}\Big)Ne^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} = \boldsymbol{p}Ne^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}.\\ &\qquad\qquad N = \Big(\frac{1}{2\pi\hbar}\Big)^{3/2}. \quad \text{(Normalization Factor)}\end{aligned}$$

2. In p-representation:

$$\begin{aligned}&\hat{\boldsymbol{x}}|\boldsymbol{x}\rangle = \boldsymbol{x}|\boldsymbol{x}\rangle, \quad \Big(i\hbar\frac{\partial}{\partial \boldsymbol{p}}\Big)Ne^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} = \boldsymbol{x}Ne^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}.\\ &\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle, \quad \hat{\boldsymbol{p}}\delta(\boldsymbol{p}-\boldsymbol{p}') = \boldsymbol{p}'\delta(\boldsymbol{p}-\boldsymbol{p}').\\ &\qquad\qquad N = \Big(\frac{1}{2\pi\hbar}\Big)^{3/2}. \quad \text{(Normalization Factor)}\end{aligned}$$

3. Commutation relation:

$$\begin{aligned}&[\hat{x}_i,\hat{p}_j] = i\hbar\delta_{ij}; \quad [\hat{x}_i,\hat{x}_j] = [\hat{p}_i,\hat{p}_j] \equiv 0.\\ &\qquad\qquad\qquad\qquad\qquad\qquad \text{vs.} \updownarrow\\ &[x_i,p_j]_{PB} = \delta_{ij}; \quad [x_i,x_j]_{PB} = [p_i,p_j]_{PB} \equiv 0.\end{aligned}$$

4. Dirac's δ-fuction:

$$\begin{aligned}&\int_{-\infty}^{+\infty} e^{\pm ikx}\mathrm{d}k = 2\pi\delta(x),\\ &\int_{-\infty}^{+\infty} e^{\pm ipx/\hbar}\mathrm{d}p = 2\pi\hbar\delta(p).\end{aligned}$$

$$\langle \boldsymbol{x}|\boldsymbol{p}\rangle = Ne^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} \quad \Rightarrow \quad \langle \boldsymbol{p}|\boldsymbol{x}\rangle = (\langle \boldsymbol{x}|\boldsymbol{p}\rangle)^* = Ne^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar},$$
$$\hat{\boldsymbol{x}}|\boldsymbol{x}\rangle = \boldsymbol{x}|\boldsymbol{x}\rangle \quad \Rightarrow \quad \hat{\boldsymbol{x}}\left(\int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\right)|\boldsymbol{x}\rangle = \left(\int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\right)\boldsymbol{x}|\boldsymbol{x}\rangle.$$

$$\left.\begin{aligned} l.h.s. &= \int \hat{\boldsymbol{x}} N e^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}|\boldsymbol{p}\rangle; \\ r.h.s. &= \int \boldsymbol{x} N e^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}|\boldsymbol{p}\rangle; \end{aligned}\right\} \quad \Rightarrow \quad \hat{\boldsymbol{x}} = i\hbar\frac{\partial}{\partial \boldsymbol{p}}.$$

$$\frac{\partial}{\partial \boldsymbol{x}} e^{+i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} = i\frac{\boldsymbol{p}}{\hbar}, \quad \Rightarrow \quad -i\hbar\frac{\partial}{\partial \boldsymbol{x}} e^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} = \boldsymbol{p}\cdot e^{+i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar},$$
$$\frac{\partial}{\partial \boldsymbol{p}} e^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} = -\frac{i}{\hbar}\boldsymbol{x}, \quad \Rightarrow \quad i\hbar\frac{\partial}{\partial \boldsymbol{p}} e^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} = \boldsymbol{x}\cdot e^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}.$$

$$N = \left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}}, \quad (\text{for 1-}D,\ N = \frac{1}{\sqrt{2\pi\hbar}}).$$

$\boldsymbol{x}$-representation	$\boldsymbol{p}$-representation
$\hat{\boldsymbol{x}}\delta(\boldsymbol{x}-\boldsymbol{x}') = \boldsymbol{x}'\delta(\boldsymbol{x}-\boldsymbol{x}')$,	$\hat{\boldsymbol{p}}\delta(\boldsymbol{p}-\boldsymbol{p}') = \boldsymbol{p}'\delta(\boldsymbol{p}-\boldsymbol{p}')$,
$\left(-i\hbar\frac{\partial}{\partial \boldsymbol{x}}\right)(Ne^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}) = \boldsymbol{p}(Ne^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar})$,	$\left(i\hbar\frac{\partial}{\partial \boldsymbol{p}}\right)(Ne^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}) = \boldsymbol{x}(Ne^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar})$,
$\begin{cases} \hat{\boldsymbol{x}} = \boldsymbol{x}, \\ \hat{\boldsymbol{p}} = -i\hbar\frac{\partial}{\partial \boldsymbol{p}}. \end{cases}$	$\begin{cases} \hat{\boldsymbol{x}} = i\hbar\frac{\partial}{\partial \boldsymbol{p}}, \\ \hat{\boldsymbol{p}} = \boldsymbol{p}. \end{cases}$
$\begin{cases} \psi_{\boldsymbol{p}}(\boldsymbol{x}) = Ne^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}, \\ \psi_{\boldsymbol{x}}(\boldsymbol{x}') = \delta(\boldsymbol{x}-\boldsymbol{x}'). \end{cases}$	$\begin{cases} \psi_{\boldsymbol{x}}(\boldsymbol{p}) = Ne^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}, \\ \psi_{\boldsymbol{p}}(\boldsymbol{p}') = \delta(\boldsymbol{p}-\boldsymbol{p}'). \end{cases}$

$$\begin{aligned} \langle \boldsymbol{x}|\boldsymbol{x}'\rangle &= \delta(\boldsymbol{x}-\boldsymbol{x}') \\ &= \langle \boldsymbol{x}|\left(\int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\right)|\boldsymbol{x}'\rangle \\ &= \int \mathrm{d}\boldsymbol{p}\langle \boldsymbol{x}|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\boldsymbol{x}'\rangle \\ &= \int \mathrm{d}\boldsymbol{p}(Ne^{i\boldsymbol{p}\cdot\boldsymbol{x}}/\hbar)(Ne^{-i\boldsymbol{p}\cdot\boldsymbol{x}'}/\hbar) \\ &= N^2\int e^{i\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{x}')/\hbar}\mathrm{d}\boldsymbol{p} \\ &= (2\pi\hbar)^3 N^2\delta(\boldsymbol{x}-\boldsymbol{x}'). \end{aligned}$$

$$\Rightarrow \quad N^2(2\pi\hbar)^3 = 1 \quad \Rightarrow \quad N^2 = \left(\frac{1}{2\pi\hbar}\right)^3 \quad \Rightarrow \quad N = \left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}}. \ (\text{let } N \in \mathbb{R} \text{ and } > 0)$$

Summary

$$\begin{cases} 1) \quad \hat{\boldsymbol{x}}|\boldsymbol{x}\rangle = \boldsymbol{x}|\boldsymbol{x}\rangle; \begin{cases} \langle \boldsymbol{x}|\boldsymbol{x}'\rangle = \delta(\boldsymbol{x}-\boldsymbol{x}'). \text{ orthonormality} \\ \int \mathrm{d}\boldsymbol{x}|\boldsymbol{x}\rangle\langle\boldsymbol{x}| = \mathbb{1}. \text{ completeness/resolution of identity} \end{cases} \\ 2) \quad \hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = \hat{\boldsymbol{p}}|\boldsymbol{p}\rangle; \begin{cases} \langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}'). \text{ orthonormality} \\ \int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \mathbb{1}. \text{ completeness/resolution of identity} \end{cases} \\ 3) \quad \begin{cases} \psi_{\boldsymbol{p}}(\boldsymbol{x}) = \langle \boldsymbol{x}|\boldsymbol{p}\rangle = \left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}} e^{i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}; \quad \hat{\boldsymbol{p}} = -i\hbar\dfrac{\partial}{\partial \boldsymbol{x}} = -i\hbar\nabla. \\ \psi^*_{\boldsymbol{p}}(\boldsymbol{x}) = \psi_{\boldsymbol{x}}(\boldsymbol{p}) = \left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}} e^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar}; \quad \hat{\boldsymbol{x}} = i\hbar\dfrac{\partial}{\partial \boldsymbol{p}} = i\hbar\nabla_{\boldsymbol{p}}. \end{cases} \end{cases}$$

Angular Momentum (Orbital)

Definition of AM:

CM: $\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}$, $\qquad \dfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{F} = \boldsymbol{N}$. ($\boldsymbol{L}$: AM, $\boldsymbol{N}$: torque)

QM: $\hat{\boldsymbol{L}} = \hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}}$. (CM $\leftrightarrow$ QM, correspondence, but only orbital AM.)

Commutation:

1. $[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k. \quad \leftarrow \quad [\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij};\ [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] \equiv 0 \leftrightarrow \hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = i\hbar\hat{\boldsymbol{L}}.$

2. $[\hat{\boldsymbol{L}^2}, \hat{L}_i] \equiv 0$. (simultaneous eigenstates).

3. $\begin{cases} [\hat{L}_i, \hat{x}_j] = i\hbar\epsilon_{ijk}\hat{x}_k. \\ [\hat{L}_i, \hat{p}_j] = i\hbar\epsilon_{ijk}\hat{p}_k. \quad \Rightarrow \quad [\hat{L}_i, \hat{\boldsymbol{p}^2}] \equiv 0. \end{cases}$

4. for $\hat{V}(\boldsymbol{x}) = V(r), \quad \left(r = (x^2+y^2+z^2)^{\frac{1}{2}}\right)$ central potential $\Rightarrow \quad [\hat{L}_i, \hat{V}(r)] \equiv 0.$

Also, for any kinetic energy: $\hat{T} = \hat{\boldsymbol{p}^2}/2m$,

$$[\hat{L}_i, \hat{T}] \equiv 0. \ \Rightarrow\ [\hat{L}_i, \hat{H}] \equiv 0. \text{ (for central potential)}$$

Eignevalue/Eigenstates:

$$[\hat{\boldsymbol{L}^2}, \hat{L}_z] \equiv 0. \quad \Rightarrow \quad \begin{cases} \hat{\boldsymbol{L}^2}|lm\rangle = \hbar^2 l(l+1)|lm\rangle, \quad (l = 0, 1, 2, \cdots), \\ \hat{L}_3|lm\rangle = m_l\hbar|lm_l\rangle. \quad (m_l = -l, \cdots, +l). \end{cases}$$

Compatible observables have simultaneous eigenstates. (相容力学量有共同本征态)

Wave function of the $(\hat{\boldsymbol{L}}^2, \hat{L}_z) \leftrightarrow |lm\rangle$

$$\langle \boldsymbol{x}|lm\rangle = \mathrm{Y}_{lm}(\theta,\phi). \Rightarrow \text{ Spherical harmonics (球谐函数)}$$

$$Y_{lm}(\theta,\phi) \sim P_l^m(\theta,\phi)e^{im\phi} \text{ are } \begin{cases}\text{orthogonal, nomalized}\\ \text{complete set of function}\end{cases}$$

$$\langle lm|l'm'\rangle = \delta_{ll'}\delta_{mm'}, \quad \sum_{l=0}^{n-1}\sum_{m=-l}^{l}|lm\rangle\langle lm| = \mathbb{1}.$$

Ladder operator (Raising/Lowering operator)

Definition:

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y = \hat{L}_1 \pm i\hat{L}_2.$$

Commutation:

1. $[\hat{L}_\pm, \hat{\boldsymbol{L}}^2] \equiv 0.$ simultaneous eigenstates
2. $[\hat{L}_x,\hat{L}_z] \pm i[\hat{L}_y,\hat{L}_z] = -i\hbar\hat{L}_y \pm i(i\hbar\hat{L}_z) = \mp\hbar\hat{L}_x - i\hbar\hat{L}_y = \mp\hbar(\hat{L}_x \pm i\hat{L}_y) = \mp\hbar\hat{L}_\pm.$
3. $\hat{L}_\pm|lm\rangle \Rightarrow |lm\pm1\rangle \begin{cases} m+1 : \text{Raising.}\\ m-1 : \text{Lowering.}\end{cases}$

$$\hat{L}_\pm\hat{L}_z - \hat{L}_z\hat{L}_\pm = \mp\hbar\hat{L}_\pm. \quad \Rightarrow \quad \hat{L}_\pm\hat{L}_z = \hat{L}_z\hat{L}_\pm \mp \hbar\hat{L}_\pm.$$

$$\Rightarrow \hat{L}_\pm\hat{L}_z|lm\rangle = \hat{L}_\pm\hat{L}_z|lm\rangle = m_l\hbar(\hat{L}_\pm|lm\rangle).$$

$$\Rightarrow (\hat{L}_z\hat{L}_\pm \mp \hbar\hat{L}_\pm)|lm\rangle = (\hat{L}_z \mp \hbar)(\hat{L}_\pm|lm\rangle).$$

$$\Rightarrow \hat{L}_z(\hat{L}_\pm|lm\rangle) = (m_l \pm 1)\hbar(\hat{L}_\pm|lm\rangle).$$

$\Rightarrow \hat{L}_\pm|lm\rangle$ is the eigenstates of $\hat{L}_z$, eigenvalue is $(m_l\pm1)\hbar$.

$\Rightarrow \hat{L}_\pm|lm\rangle \sim |lm\pm1\rangle$.

Actually,

$$\hat{L}_\pm|lm_l\rangle = \hbar\sqrt{l(l+1) - m_l(m_l\pm1)}|lm_l\pm1\rangle.$$

Similarly,

$$\hat{S}_\pm|sm_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s\pm1)}|sm_s\pm1\rangle.$$

for single 1/2-spin system, $m_s = -1/2, +1/2$.

$$\Longrightarrow \qquad \hat{S}_{\pm}\Big|-\frac{1}{2}\Big\rangle = \hbar\sqrt{\frac{1}{2}\Big(\frac{1}{2}+1\Big)-\Big(-\frac{1}{2}\Big)\Big(-\frac{1}{2}+1\Big)}\Big|-\frac{1}{2}+1\Big\rangle = \hbar\Big|+\frac{1}{2}\Big\rangle;$$
$$\hat{S}_{-}\Big|+\frac{1}{2}\Big\rangle = \hbar\sqrt{\frac{1}{2}\Big(\frac{1}{2}+1\Big)-\Big(\frac{1}{2}\Big)\Big(\frac{1}{2}-1\Big)}\Big|\frac{1}{2}-1\Big\rangle = \hbar\Big|-\frac{1}{2}\Big\rangle.$$

let

$$\hat{S}_{\pm} = \hbar\hat{\sigma}_{\pm}, \quad \Rightarrow \quad \sigma_{\pm}\begin{cases}\hat{\sigma}_{+}\Big|-\frac{1}{2}\Big\rangle = |+\rangle;\\ \hat{\sigma}_{-}\Big|+\frac{1}{2}\Big\rangle = |-\rangle.\end{cases}$$

let

$$\begin{cases}\Big|-\frac{1}{2}\Big\rangle = |\downarrow\rangle = |-\rangle = |1\rangle = \begin{pmatrix}0\\1\end{pmatrix} \Rightarrow \hat{\sigma}_{+}|1\rangle = |0\rangle, \hat{\sigma}_{+} = |0\rangle\langle 1|.\\ \Big|+\frac{1}{2}\Big\rangle = |\uparrow\rangle = |+\rangle = |0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \Rightarrow \hat{\sigma}_{-}|0\rangle = |1\rangle, \hat{\sigma}_{-} = |1\rangle\langle 0|.\end{cases}$$

$\hat{\sigma}_{\pm}$: ladder operator (transition operator).

$$\left.\begin{aligned}\hat{S}_{\pm} = \hat{S}_x \pm i\hat{S}_y = \frac{\hbar}{2}(\hat{\sigma}_x \pm i\hat{\sigma}_y)\\ \hat{S}_{\pm} = \hbar\hat{\sigma}_x\end{aligned}\right\} \Rightarrow \hat{\sigma}_{\pm} = \frac{1}{2}(\hat{\sigma}_x \pm i\hat{\sigma}_y).$$

Exercises: 1. Prove the following commutation relations:

$$[\hat{\boldsymbol{J}}^2, J_{\pm}] = 0;$$
$$[\hat{J}_x, J_{\pm}] = \mp\hbar J_z;$$
$$[\hat{J}_y, J_{\pm}] = -i\hbar J_z;$$
$$[\hat{J}_z, \hat{J}_{\pm}] = \pm\hbar J_{\pm};$$
$$[\hat{J}_{+}, \hat{J}_{-}] = 2\hbar J_z.$$

Lecture Notes 9 Spin and Pauli Matrix

Contents

- Ladder operators (Raising and Lowering operators);
- Spin angular momentum;
- Pauli operator (matrix).

Ladder operators of spin

1.
$$\begin{aligned}\hat{S}_\pm|s,m_s\rangle &= \hbar\sqrt{s(s+1)-m_s(m_s\pm1)}|s,m_s\pm1\rangle \\ &= \hbar\sqrt{s(s+1)-m_s(m_s\pm1)}|m_s\pm1\rangle.\end{aligned}$$

2. For single spin-1/2, $s=1/2$, $m_s=\pm1/2$.

$$\Longrightarrow \quad \begin{cases}\hat{S}_+\Big|-\frac{1}{2}\Big\rangle = \hbar\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)-\left(-\frac{1}{2}\right)\left(-\frac{1}{2}+1\right)}\Big|-\frac{1}{2}+1\Big\rangle = \hbar\Big|+\frac{1}{2}\Big\rangle, \\ \hat{S}_-\Big|+\frac{1}{2}\Big\rangle = \hbar\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)-\left(\frac{1}{2}\right)\left(\frac{1}{2}-1\right)}\Big|\frac{1}{2}-1\Big\rangle = \hbar\Big|-\frac{1}{2}\Big\rangle.\end{cases}$$

$$\Longrightarrow \qquad \hat{S}_+|\downarrow\rangle = \hbar|\uparrow\rangle, \quad \hat{S}_-|\uparrow\rangle = \hbar|\downarrow\rangle, \quad \hat{S}_\pm = \hbar\hat{\sigma}_\pm.$$

$$\hat{\sigma}_+|\downarrow\rangle = |\uparrow\rangle, \quad \hat{\sigma}_-|\uparrow\rangle = |\downarrow\rangle.$$

let
$$\begin{cases}|\uparrow\rangle = |+\rangle = \Big|+\frac{1}{2}\Big\rangle = |0\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \\ |\downarrow\rangle = |-\rangle = \Big|-\frac{1}{2}\Big\rangle = |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}.\end{cases}$$

$$\Longrightarrow \qquad \begin{cases}\hat{\sigma}_+|1\rangle = |0\rangle, \ \hat{\sigma}_-|0\rangle = |1\rangle, \\ \hat{\sigma}_+|0\rangle = 0, \ \hat{\sigma}_-|1\rangle = 0.\end{cases}$$

where

$$\hat{\sigma}_+ = \mathbb{1}\hat{\sigma}_+\mathbb{1} = \big(|0\rangle\langle 0| + |1\rangle\langle 1|\big)\hat{\sigma}_+\big(|0\rangle\langle 0| + |1\rangle\langle 1|\big) = |0\rangle\langle 1|.$$

Similarly, one has

$$\hat{\sigma}_- = |1\rangle\langle 0|.$$

Spin angular momentum:

Definition:

$$\left[\hat{S}_i, \hat{S}_j\right] = i\hbar\epsilon_{ijk}\hat{S}_k \Leftrightarrow \hat{\boldsymbol{S}} \times \hat{\boldsymbol{S}} = i\hbar\hat{\boldsymbol{S}}.$$

Properties of Spin angular momentum:

For single 1/2-spin system: $\hat{\boldsymbol{S}}^2 = \frac{3}{4}\hbar^2 \cdot \mathbb{1}_2; \quad \hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z.$

$$\hat{\boldsymbol{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}. \qquad \hat{\boldsymbol{\sigma}} \text{ : Pauli vector}$$

$$\Longrightarrow \quad [\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k. \qquad \hat{\boldsymbol{\sigma}} = \hat{\sigma}_i\hat{e}_i, \quad \hat{\sigma}_i \text{ : Pauli operator (Pauli matrix)}$$

$$\hat{\boldsymbol{S}}^2 = \frac{3}{4}\hbar^2 \cdot \mathbb{1}_2; \quad \hat{S}_i^2 = \frac{\hbar^2}{4} \cdot \mathbb{1}_2; \implies \hat{\boldsymbol{\sigma}}^2 = 3 \cdot \mathbb{1}_2; \quad \hat{\sigma}_i^2 = \mathbb{1}_2.$$

Eigenvalue/eigenstates:

For single spin-1/2, $s = \frac{1}{2},\ m_s = -\frac{1}{2}, +\frac{1}{2}; \quad |0\rangle = |\uparrow\rangle = |+\rangle,\ |1\rangle = |\downarrow\rangle = |-\rangle.$

Orthonormality and resolution of identity:

$$\begin{cases} \langle 0|1\rangle = \langle 1|0\rangle = 0, \\ \langle 0|0\rangle = \langle 1|1\rangle = 1, \\ |0\rangle\langle 0| + |1\rangle\langle 1| = \mathbb{1}_2. \end{cases}$$

Eigenvalue equations:

$$\begin{cases} \hat{\boldsymbol{S}}^2|s, m_s\rangle = s(s+1)\hbar^2|s, m_s\rangle, \\ \hat{S}_z|s, m_s\rangle = m_s\hbar|s, m_s\rangle. \end{cases}$$

$$\Longrightarrow \quad \begin{cases} \hat{\boldsymbol{S}}^2|0\rangle = \frac{3}{4}\hbar^2|0\rangle, \\ \hat{S}_z|0\rangle = \frac{\hbar}{2}|0\rangle. \end{cases} \quad \begin{cases} \hat{\boldsymbol{S}}^2|1\rangle = \frac{3}{4}\hbar^2|1\rangle, \\ \hat{S}_z|1\rangle = -\frac{\hbar}{2}|1\rangle. \end{cases}$$

$$\Longrightarrow \quad \begin{cases} \hat{\boldsymbol{\sigma}}^2|0\rangle = 3|0\rangle, \\ \hat{\sigma}_z|0\rangle = |0\rangle. \end{cases} \quad \begin{cases} \hat{\boldsymbol{\sigma}}^2|1\rangle = 3|1\rangle, \\ \hat{\sigma}_z|1\rangle = -|1\rangle. \end{cases}$$

Pauli matrices $\hat{\sigma}_z = \mathbb{1}\hat{\sigma}_z\mathbb{1} = (|0\rangle\langle 0| + |1\rangle\langle 1|)\,\hat{\sigma}_z\,(|0\rangle\langle 0| + |1\rangle\langle 1|) = |0\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

$$\hat{\sigma}_\pm = (\hat{\sigma}_x \pm i\hat{\sigma}_y)/2 = \begin{cases} \hat{\sigma}_+ = |0\rangle\langle 1| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \\ \hat{\sigma}_- = |1\rangle\langle 0| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \end{cases}$$

$$\Longrightarrow \quad \begin{cases} \hat{\sigma}_x = \hat{\sigma}_+ + \hat{\sigma}_- = |0\rangle\langle 1| + |1\rangle\langle 0| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \hat{\sigma}_y = -i\,(\hat{\sigma}_+ - \hat{\sigma}_-) = -i\,(|0\rangle\langle 1| - |1\rangle\langle 0|) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \end{cases}$$

$$\Longrightarrow \quad \begin{cases} \hat{\sigma}_1 = \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \hat{\sigma}_2 = \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \hat{\sigma}_3 = \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \\ \hat{\sigma}_0 = \mathbb{1}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \hat{\sigma}_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad \hat{\sigma}_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; \quad \hat{\boldsymbol{\sigma}}^2 = 3 \cdot \mathbb{1}_2 = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}. \end{cases}$$

($\forall\ \boldsymbol{M}_{2\times 2},$ one has $\boldsymbol{M}_{2\times 2} = a_\alpha\hat{\sigma}_\alpha = a_0\hat{\sigma}_0 + \boldsymbol{a}\cdot\hat{\boldsymbol{\sigma}}$.)

Compare:

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y = \frac{\hbar}{2}(\hat{\sigma}_x \pm i\hat{\sigma}_y).$$

Also, $\hat{S}_\pm = \hbar\hat{\sigma}_\pm$, so, $\hat{\sigma}_\pm = \frac{1}{2}(\hat{\sigma}_x \pm i\hat{\sigma}_y)$.

Properties of Pauli Matrices:

a) General expression of Pauli matrices:

$$\hat{\sigma}_k = \begin{pmatrix} \delta_{k3} & \delta_{k1} - i\delta_{k2} \\ \delta_{k1} + i\delta_{k2} & -\delta_{k3} \end{pmatrix}, \quad (k = 1, 2, 3).$$

$$\hat{\boldsymbol{\sigma}} = \boldsymbol{e}_k\hat{\sigma}_k. \quad (k = 1, 2, 3).$$

b) Commutations/Anti-Commutations:

$$\hat{\sigma}_i\hat{\sigma}_j = \delta_{ij}\mathbb{1}_2 + i\epsilon_{ijk}\hat{\sigma}_k \Rightarrow \begin{cases} \hat{\sigma}_i^2 = \mathbb{1}_2, & (i=j) \\ \hat{\sigma}_i\hat{\sigma}_j = i\epsilon_{ijk}\sigma_k. & (i\neq j) \end{cases}$$

$$\Rightarrow \begin{cases} [\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k, \\ \{\hat{\sigma}_i, \hat{\sigma}_j\} = 2\delta_{ij}\mathbb{1}_2. \end{cases}$$

Exercises:

1. Prove the Pauli matrices have the following properties:

(1) $\begin{cases} [\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k; \\ \{\hat{\sigma}_i, \hat{\sigma}_j\} = 2\delta_{ij}1_2; \end{cases}$

(2) $\mathrm{Tr}(\hat{\sigma}_i) = 0;$

(3) $\det(\hat{\sigma}_i) = -1;$

(4) $\hat{\sigma}_i^2 = \mathbb{1}_2, \quad \hat{\boldsymbol{\sigma}}^2 = 3\cdot\mathbb{1}_2;$

(5) $\det(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{A}) = -\boldsymbol{A}^2.$

2. Prove that for all 2×2 matrices $\boldsymbol{M}_{2\times 2}$, it can always be expressed as $\boldsymbol{M}_{2\times 2} = a_0\hat{\sigma}_0 + \hat{\boldsymbol{a}}\hat{\boldsymbol{\sigma}}$.

3. Derive $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ from its definition of spin.

Lecture Notes 10 Ladder Operators and Algebraic Method in QM

Contents

- Ladder operators and commutation relations;
- Algebraic method in QM.

General Definition of Angular Momentum in QM

$\boxed{[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}, \quad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] \equiv 0.}$ $\Longleftarrow$ Foundamental Commutation Relations

$\Big\Downarrow \hat{L}_i = (\hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}})_i = \epsilon_{ijk}\hat{x}_j\hat{p}_k.$

$\boxed{[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k} \Longrightarrow \boxed{[\hat{\boldsymbol{L}}^2, \hat{L}_i] \equiv 0.}$

$$\Longrightarrow \begin{cases} \boxed{\hat{L}_\pm = \hat{L}_1 \pm i\hat{L}_2.} \text{ Ladder Operators} \\ [\hat{\boldsymbol{L}}^2, \hat{L}_1] = [\hat{\boldsymbol{L}}^2, \hat{L}_2] \equiv 0 \Longrightarrow \boxed{[\hat{\boldsymbol{L}}^2, \hat{L}_\pm] \equiv 0.} \\ \boxed{[\hat{\boldsymbol{L}}^2, \hat{L}_z] \equiv 0.} \Rightarrow \text{common eigenstates } |lm \end{cases}$$

$\Big\Downarrow$ Similarly, we can define the spin:

$\boxed{[\hat{S}_i, \hat{S}_j] = i\hbar\epsilon_{ijk}\hat{S}_k} \Longrightarrow \boxed{[\hat{\boldsymbol{S}}^2, \hat{S}_i] \equiv 0.}$

$$\Longrightarrow \begin{cases} \boxed{\hat{S}_\pm = \hat{S}_1 \pm i\hat{S}_2.} \\ [\hat{\boldsymbol{S}}^2, \hat{S}_1] = [\hat{\boldsymbol{S}}^2, \hat{S}_i] \equiv 0 \Longrightarrow \boxed{[\hat{S}^2, \hat{S}_\pm] \equiv 0.} \\ \boxed{[\hat{\boldsymbol{S}}^2, \hat{S}_z] \equiv 0.} \Rightarrow \text{common eigenstates } |sm \end{cases}$$

$\Big\Downarrow$ Spin has no classical counterpart.

$\boxed{\hat{\boldsymbol{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}} \Longrightarrow \hat{S}_i = \frac{\hbar}{2}\hat{\sigma}_i.}$

$$\boxed{\hat{\sigma}_i\hat{\sigma}_j = \delta_{ij}\mathbb{1}_2 + i\epsilon_{ijk}\hat{\sigma}_k.} \Longrightarrow \begin{cases} [\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k, \\ \{\hat{\sigma}_i, \hat{\sigma}_j\} = 2\delta_{ij}\mathbb{1}_2, \\ \hat{\sigma}_i^2 \equiv \mathbb{1}_2, \ \hat{\boldsymbol{\sigma}}^2 = 3 \cdot \mathbb{1}_2. \end{cases} \Longrightarrow \boxed{\begin{array}{l} \hat{\sigma}_\pm = \frac{1}{2}(\hat{\sigma}_1 \pm i\hat{\sigma}_2), \\ \hat{S}_\pm = \hbar\hat{\sigma}_\pm. \end{array}}$$

$$\boxed{\hat{\boldsymbol{J}}=\hat{\boldsymbol{L}}+\hat{\boldsymbol{S}}} \Longrightarrow \boxed{\hat{J}_i=\hat{L}_i+\hat{S}_i.} \qquad \Longrightarrow \boxed{\begin{cases}\hat{J}_\pm=\hat{J}_1\pm i\hat{J}_2,\\ [\hat{J}_\pm,\hat{\boldsymbol{J}}^2]\equiv 0.\end{cases}}$$

$$\Longrightarrow \boxed{[\hat{J}_i,\hat{J}_j]=i\hbar\epsilon_{ijk}\hat{J}_k} \Longrightarrow \boxed{[\hat{\boldsymbol{J}}^2,\hat{J}_i]\equiv 0.} \quad \Longrightarrow \begin{cases}\hat{\boldsymbol{J}}^2|jm_j\rangle=j(j+1)\hbar^2|jm_j\rangle,\\ \hat{J}_z|jm_j\rangle=m_j\hbar|jm_j\rangle,\\ j\text{: azimuthal quantum number (角量子数)},\\ m_j\text{: magnetic quantum number (磁量子数)}.\end{cases}$$

$$\begin{cases}L\text{: orbital (outer)},\\ S\text{: spin (intrinsic)}.\end{cases} \Longrightarrow \boxed{[\hat{L}_i,\hat{S}_j]\equiv 0.} \qquad \boxed{[\hat{J}_i,\hat{J}_j]=i\hbar\epsilon_{ijk}\hat{J}_k} \Longrightarrow \text{ General Definition for AM.}$$

where J can be orbital/spin/total/arbitrary AM.

Consider interaction with a magnetic field $\begin{cases}(\hat{H}_I)_O=-\dfrac{q}{2mc}\hat{\boldsymbol{L}}\cdot\boldsymbol{B}=-\dfrac{q}{2mc}\hat{L}_zB_z.\\ (\hat{H}_I)_S=-\dfrac{q}{2mc}\hat{\boldsymbol{S}}\cdot\boldsymbol{B}=-\dfrac{q}{mc}\hat{S}_zB_z.\end{cases}$

Derivation of an important formula

We have introduced the Ladder Operator (Raising/Lowering Operator), now let's derive an important formula of Ladder Operator, which is:

$$\boxed{\hat{J}_\pm|jm_j\rangle=\hbar\sqrt{j(j+1)-m_j(m_j\pm 1)}|jm_j\pm 1\rangle.}$$

To derive this formula, we first revisit some commutation relations.

1) $[\hat{J}_\pm,\hat{\boldsymbol{J}}^2]\equiv 0 \Longrightarrow [\hat{J}_\pm^n,\hat{\boldsymbol{J}}^2]\equiv 0.$
   $[\hat{J}_3,\hat{\boldsymbol{J}}^2]\equiv 0.$
2) $[\hat{J}_\pm,\hat{J}_3]=\mp\hbar\hat{J}_\pm,$
   $\Longrightarrow \boxed{\hat{J}_3\hat{J}_\pm=\hat{J}_\pm\hat{J}_3\pm\hbar\hat{J}_\pm.}$
3) $\begin{cases}\hat{J}_+\hat{J}_-=\hat{\boldsymbol{J}}^2-\hat{J}_3^2+\hbar\hat{J}_3.\\ \hat{J}_-\hat{J}_+=\hat{\boldsymbol{J}}^2-\hat{J}_3^2-\hbar\hat{J}_3.\end{cases}$

$$\begin{aligned}[\hat{J}_\pm,\hat{J}_3] &= [\hat{J}_1\pm i\hat{J}_2,\hat{J}_3]\\ &= [\hat{J}_1,\hat{J}_3]\pm i[\hat{J}_2,\hat{J}_3]\\ &= -i\hbar\hat{J}_2\pm i(i\hbar)\hat{J}_1\\ &= \mp\hbar(\hat{J}_1\pm i\hat{J}_2)=\mp\hat{J}_\pm.\end{aligned}$$

$$\begin{aligned}\hat{J}_\pm\hat{J}_\mp &= (\hat{J}_1\pm i\hat{J}_2)(\hat{J}_1\mp i\hat{J}_2)\\ &= \hat{J}_1^2\mp i\hat{J}_1\hat{J}_2\pm i\hat{J}_2\hat{J}_1+\hat{J}_2^2\\ &= \hat{\boldsymbol{J}}^2-\hat{J}_3^2\mp i[\hat{J}_1,\hat{J}_2]\\ &= \hat{\boldsymbol{J}}^2-\hat{J}_3^2\mp i\cdot i\hbar\hat{J}_3\\ &= \hat{\boldsymbol{J}}^2-\hat{J}_3^2\pm\hat{J}_3.\end{aligned}$$

1. Suppose

$$\begin{cases} \hat{\boldsymbol{J}}^2|\lambda m\rangle = \hbar^2\lambda|\lambda m\rangle, \\ \hat{J}_3|\lambda m\rangle = \hbar m|\lambda m\rangle. \end{cases}$$

Then we have

$$\begin{aligned} & \hat{J}_3(\hat{J}_\pm|\lambda m\rangle) \\ = \; & (\hat{J}_\pm\hat{J}_3 \pm \hbar\hat{J}_\pm)|\lambda m\rangle \\ = \; & \hbar m\hat{J}_\pm|\lambda m\rangle \pm \hbar\hat{J}_\pm|\lambda m\rangle = \hbar(m\pm 1)(\hat{J}_\pm|\lambda m\rangle). \end{aligned}$$

This indicates that $\hat{J}_\pm|\lambda m\rangle$ are the eigenstates of $\hat{J}_z$, with the eigenvalues of $(m\pm 1)\hbar$.

Hence,

$$\hat{J}_\pm|\lambda m\rangle = C_\pm|\lambda m\pm 1\rangle,$$

and,

$$\hat{J}_\pm^n|\lambda m\rangle = D_\pm|\lambda m\pm n\rangle.$$

2. $\langle\hat{\boldsymbol{J}}^2\rangle = \lambda\hbar^2, \quad \langle\hat{J}_3^2\rangle = m^2\hbar^2.$

Since we have $m^2\hbar^2 = \langle\hat{J}_3^2\rangle \le \langle\hat{\boldsymbol{J}}^2\rangle = \lambda\hbar^2 \Longrightarrow \boxed{m^2 \le \lambda, \quad \lambda \ge 0.}$.

This is the confinement of m in terms of λ.

3. Since $\exists$ interger $m_0 \Longrightarrow \hat{J}_-|\lambda m_0\rangle = 0$.

$\exists$ integer $N \ge 0 \Longrightarrow \hat{J}_+|\lambda m_0 + N\rangle = 0$.

1) Since $\hat{J}_+\hat{J}_-|\lambda m_0\rangle \equiv 0$, and

$$\begin{aligned} \hat{J}_-\hat{J}_+|\lambda, m_0\rangle = \; & (\hat{\boldsymbol{J}}^2 - \hat{J}_3^2 + \hbar\hat{J}_3)|\lambda m_0\rangle \\ = \; & \hbar^2\big(\lambda - m_0^2 + m_0\big)|\lambda m_0\rangle. \\ \Longrightarrow \; & \boxed{\lambda - m_0^2 + m_0 = 0.} \end{aligned}$$

2) Since $\hat{J}_-\hat{J}_+|\lambda, m_0+N\rangle = 0$, and

$$\begin{aligned} \hat{J}_-\hat{J}_+|\lambda, m_0+N\rangle = \; & (\hat{\boldsymbol{J}}^2 - \hat{J}_3^2 - \hbar\hat{J}_3^2)|\lambda, m_0+N\rangle. \\ = \; & \hbar^2\big[\lambda - (m_0+N)^2 - (m_0+N)\big]|\lambda, m_0+N\rangle. \\ \Longrightarrow \; & \boxed{\lambda - (m_0+N)^2 - (m_0+N) = 0.} \end{aligned}$$

Now we have：

$$\begin{cases}\lambda-(m_0+N)^2-(m_0+N)=0.\\ \lambda-m_0^2+m_0=0.\end{cases}$$

$$\begin{aligned}\Longrightarrow\quad & -(m_0^2+2m_0N+N^2)+m_0^2-(m_0+N)-m_0=0.\\ & -2m_0N-N^2-2m_0-N=0.\\ & -(2m_0+N)(N+1)=0.\end{aligned}$$

$$\Longrightarrow\quad\begin{cases}m_0=-\dfrac{N}{2},\ m_0+N=+\dfrac{N}{2}.\\ \lambda=(m_0+N)^2+(m_0+N)=\dfrac{N}{2}\Big(\dfrac{N}{2}+1\Big).\end{cases}$$

Let $\lambda=j(j+1)$, where $j=\dfrac{N}{2},\quad (N\geq 0,\text{ integer})$, one has

$$\begin{cases}\hat{\boldsymbol{J}}^2|jm_j\rangle=\hbar^2j(j+1)|jm_j\rangle,\\ \hat{J}_3|jm_j\rangle=\hbar m_j|jm_j\rangle.\end{cases}$$

Further we find that:

$$\begin{cases}j=\dfrac{N}{2}=0,\dfrac{1}{2},1,\dfrac{3}{2},2,\cdots\quad\begin{cases}\text{integer }(\geq 0)\\ \text{odd-integer }(>0)\end{cases}\\ m_j=m_0,m_0+1,\cdots,m_0+N-1,m_0+N\\ -j,-j+1,\cdots,j-1,j.\ (2j+1)\text{-fold-degeneracy}\end{cases}$$

$$\Longrightarrow\qquad\{|jm_j\rangle\}=\begin{pmatrix}|j,-j\rangle\\ |j,-j+1\rangle\\ \vdots\\ |j,j-1\rangle\\ |j,j\rangle\end{pmatrix}.$$

Note that :

$$\begin{cases}\hat{J}_+^\dagger=(\hat{J}_1+i\hat{J}_2)^\dagger=\hat{J}_1-i\hat{J}_2=\hat{J}_-,\\ \hat{J}_-^\dagger=\hat{J}_+,\end{cases}$$

$$\begin{cases}\hat{J}_\pm\hat{J}_\mp=\hat{\boldsymbol{J}}^2-\hat{J}_3^2\pm\hbar\hat{J}_3,\\ \hat{J}_\mp\hat{J}_\pm=\hat{\boldsymbol{J}}^2-\hat{J}_3^2\mp\hbar\hat{J}_3.\end{cases}$$

So,

$$\langle jm_j|jm_j\rangle = \langle jm_j\pm1|jm_j\pm1\rangle = |C_\pm|^2 = 1.$$

Since

$$\begin{aligned}
&\langle jm_j\pm1|jm_j\pm1\rangle \\
=&\langle jm_j|\hat{J}_\mp\hat{J}_\pm|jm_j\rangle \\
=&\langle jm_j|(\hat{\boldsymbol{J}}^2 - \hat{J}_3^2 \mp \hbar\hat{J}_3)|jm_j\rangle \\
=&\hbar^2[j(j+1) - m_j^2 \mp m_j] \\
=&\hbar^2[j(j+1) - m_j(m_j \pm 1)],
\end{aligned}$$

one has

$$\boxed{\hat{J}_\pm|jm_j\rangle = \hbar\sqrt{j(j+1) - m_j(m_j\pm1)}|jm_j\pm1\rangle.}$$

where

$$\begin{cases}
(m_j)_{\max} = j, \text{ i.e.,} \quad \hat{J}_+|jj\rangle \equiv 0. \\
(m_j)_{\min} = -j, \text{ i.e.,} \quad \hat{J}_-|j\,-j\rangle \equiv 0.
\end{cases}$$

In conclusion, for arbitrary angular momentum (AM) (orbital/spin/total/ $\cdots$), one has:

$$\begin{cases}
[\hat{J}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k, \\
\hat{J}_\pm = \hat{J}_1 \pm i\hat{J}_2, \\
\begin{cases}
\hat{\boldsymbol{J}}^2|jm_j\rangle = \hbar^2 j(j+1)|jm_j\rangle, \\
\hat{J}_3|jm_j\rangle = \hbar m_j|jm_j\rangle.
\end{cases} \\
\hat{J}_\pm|jm_j\rangle = \hbar\sqrt{j(j+1) - m_j(m_j\pm1)}|jm_j\pm1\rangle.
\end{cases}$$

Commutation Relations of AM:

1)

$$\begin{cases} [\hat{L}_i,\hat{L}_j]=i\hbar\epsilon_{ijk}\hat{L}_k \Rightarrow \begin{cases} [\hat{L}_i,\hat{\boldsymbol{L}}^2]\equiv 0, \\ [\hat{L}_i,\hat{x}_j]=i\hbar\epsilon_{ijk}\hat{x}_k, \\ [\hat{L}_i,\hat{p}_k]=i\hbar\epsilon_{ijk}\hat{p}_k. \end{cases} \\ [\hat{S}_i,\hat{S}_j]=i\hbar\epsilon_{ijk}\hat{S}_k. \\ [\hat{J}_i,\hat{J}_j]=i\hbar\epsilon_{ijk}\hat{J}_k. \quad ([\hat{L}_i,\hat{S}_j]\equiv 0.) \end{cases}$$

$$\begin{aligned} &[\hat{L}_i,\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}]=[\hat{L}_i,\hat{L}_j\hat{S}_j] \\ =&[\hat{L}_i,\hat{L}_j]\hat{S}_j=i\hbar\epsilon_{ijk}\hat{L}_k\hat{S}_j\neq 0; \\ &[\hat{J}_i,\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}]=[\hat{L}_i+\hat{S}_i,\hat{L}_j\hat{S}_j] \\ =&i\hbar\epsilon_{ijk}\hat{L}_k\hat{S}_j+i\hbar\epsilon_{ijk}\hat{L}_j\hat{S}_k \\ =&i\hbar\epsilon_{ijk}(\hat{L}_k\hat{S}_j+\hat{L}_j\hat{S}_k)\equiv 0. \\ &[\hat{\boldsymbol{L}}^2,\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}] \\ =&\hat{L}_i[\hat{L}_i,\hat{L}_j]\hat{S}_j+[\hat{L}_i,\hat{L}_j]\hat{L}_i\hat{S}_j \\ =&i\hbar\epsilon_{ijk}(\hat{L}_i\hat{L}_k+\hat{L}_k\hat{L}_i)\hat{S}_j. \\ &[\hat{L}_i,\hat{\boldsymbol{p}}^2]=[\hat{L}_i,\hat{p}_j\hat{p}_j] \\ =&i\hbar\epsilon_{ijk}(\hat{p}_k\hat{p}_j+\hat{p}_j\hat{p}_k)\equiv 0. \\ &\text{Analogously, } [\hat{S}_i,\hat{\boldsymbol{p}}^2]\equiv 0. \end{aligned}$$

2) $[\hat{J}_i,\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}]\equiv 0. \leftrightarrow m_j$

3) $[\hat{\boldsymbol{L}}^2,\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}]\equiv 0 \leftrightarrow l$

4) $[\hat{\boldsymbol{S}}^2,\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}]\equiv 0 \leftrightarrow s$

5) $[\hat{\boldsymbol{J}}^2,\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}]\equiv 0 \leftrightarrow j$

Commutation Relations with Hamiltonian:

$$\hat{H}=\hat{T}(\hat{\boldsymbol{p}})+V(r)+\hat{H}_{\text{L-S}}.$$

$$\hat{T}(\hat{\boldsymbol{p}})=\frac{\hat{\boldsymbol{p}}^2}{2m},\quad \hat{V}(r)=\hat{V}(r),\quad (r=\sqrt{x^2+y^2+z^2}).$$

$$\hat{H}_{\text{L-S}}=\zeta(r)\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}.$$

$$\begin{cases} [\hat{L}_i,\hat{\boldsymbol{p}}^2]\equiv 0;\ [\hat{L}_i,\hat{V}(r)]\equiv 0. \\ [\hat{L}_i,\hat{V}(r)]=[\hat{L}_i,\hat{x}_j]\dfrac{\mathrm{d}V}{\mathrm{d}r}\dfrac{\hat{x}_j}{r}=\dfrac{i\hbar V'}{r}\epsilon_{ijk}\hat{x}_k\hat{x}_j\equiv 0. \\ [\hat{S}_i,\hat{V}(r)]\equiv 0. \end{cases}$$

$(\hat{\boldsymbol{J}}^2,\hat{J}_3,\hat{\boldsymbol{L}}^2,\hat{\boldsymbol{S}}^2)$ (conserved observable) all commute with $\hat{H}$: $[\hat{A},\hat{H}]\equiv 0$. $A=\{\hat{\boldsymbol{J}}^2,\hat{J}_3,\hat{\boldsymbol{L}}^2,\hat{\boldsymbol{S}}^2\}$ is the complete set of commuting observables (CSCO) (力学量完全集).

Summary:

$$\hat{H}=\underline{\hat{T}(\hat{\boldsymbol{p}})+\hat{V}(r)}+\underline{\xi(r)\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}}.$$

Non-Relativistic (NR) and Relativestic (R, weak relativstic) Terms:

$$\text{NR}: \quad \begin{cases} \hat{T}(\hat{\boldsymbol{p}}) = \dfrac{\hat{\boldsymbol{p}}^2}{2m} = -\dfrac{\hbar^2\nabla^2}{2m}, \\ \hat{V}(r) = \hat{V}(r), \quad (r = \sqrt{x^2+y^2+z^2}). \end{cases}$$

$$[\hat{L}_i, \hat{T}(\hat{\boldsymbol{p}})] = [\hat{L}_i, \hat{V}(r)] \equiv 0 \Longrightarrow [\hat{L}_i, \hat{T}(\hat{\boldsymbol{p}}) + \hat{V}(r)] \equiv 0.$$

$$\text{R}: \quad \xi(r)\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}},$$

$$[\hat{J}_i, \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}] = [\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}] = [\hat{\boldsymbol{L}}^2, \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}] = [\hat{\boldsymbol{S}}^2, \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}] \equiv 0.$$

$$\text{While:} \quad \begin{cases} [\hat{L}_i, \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}] \neq 0, \\ [\hat{S}_i, \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}] \neq 0. \end{cases}$$

$$\Longrightarrow (j, m_j, l, s). \quad \text{(good quantum numbers, 好量子数)}$$

$$\text{for fixed } s = \frac{1}{2}, \quad \Longrightarrow |jm_jls\rangle = |jlm_j\rangle.$$

Exercises: 1. Prove all the commutation relations in this lecture.

Lecture Notes 11 Addition of angular momenta and Clebsch-Gordan coefficients

Contents

- Clebsch-Gordan (C-G) coefficients;
- Fundamentals of the addition of angular momenta;
- Coupling and non-coupling representations.

C-G coefficients:

Definition of C-G coefficients:

Expansion coefficients of total angular momentum eigenstates in non-coupling basis (tensor product states).

Addition of two angular momenta: $|j_1 m_1\rangle \otimes |j_2 m_2\rangle \Longrightarrow |j_1 j_2 j m\rangle$.

Example:

$$j_1 = s_1 = \frac{1}{2},\ j_2 = s_2 = \frac{1}{2};\ j_1 = \frac{1}{2}\begin{cases} m_1 = -1/2 \\ m_2 = +1/2 \end{cases};\quad j_2 = \frac{1}{2}\begin{cases} m_1 = -1/2 \\ m_2 = +1/2 \end{cases}.$$

- Non-coupling representation (Tensor product basis):

$$|j_1 m_1\rangle \otimes |j_2 m_2\rangle = \begin{cases} |\uparrow\rangle_1 \otimes |\uparrow\rangle_2 = |0\rangle_1 \otimes |0\rangle_2 = \left|\frac{1}{2}\right\rangle_1 \otimes \left|\frac{1}{2}\right\rangle_2, \\ |\uparrow\rangle_1 \otimes |\downarrow\rangle_2 = |0\rangle_1 \otimes |1\rangle_2 = \left|\frac{1}{2}\right\rangle_1 \otimes \left|-\frac{1}{2}\right\rangle_2, \\ |\downarrow\rangle_1 \otimes |\uparrow\rangle_2 = |1\rangle_1 \otimes |0\rangle_2 = \left|-\frac{1}{2}\right\rangle_1 \otimes \left|\frac{1}{2}\right\rangle_2, \\ |\downarrow\rangle_1 \otimes |\downarrow\rangle_2 = |1\rangle_1 \otimes |1\rangle_2 = \left|-\frac{1}{2}\right\rangle_1 \otimes \left|-\frac{1}{2}\right\rangle_2. \end{cases}$$

- Coupling representation:

$$|j_1 j_2 jm\rangle = \begin{cases} |00\rangle = C^0_{\frac{1}{2},-\frac{1}{2}} \left|\frac{1}{2}-\frac{1}{2}\right\rangle + C^0_{-\frac{1}{2},\frac{1}{2}} \left|-\frac{1}{2}\frac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}(|0\rangle_1 \otimes |1\rangle_2 - |1\rangle_1 \otimes |2\rangle_2), \\ |1-1\rangle = C^1_{-\frac{1}{2},-\frac{1}{2}} \left|-\frac{1}{2}-\frac{1}{2}\right\rangle = |1\rangle_1 \otimes |1\rangle_2, \\ |10\rangle = C^1_{\frac{1}{2},-\frac{1}{2}} \left|\frac{1}{2}-\frac{1}{2}\right\rangle + C^1_{-\frac{1}{2}\frac{1}{2}} \left|-\frac{1}{2}\frac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}(|0\rangle_1 \otimes |1\rangle_2 + |1\rangle_2 \otimes |0\rangle_2), \\ |11\rangle = C^1_{\frac{1}{2},\frac{1}{2}} \left|\frac{1}{2}\frac{1}{2}\right\rangle = |0\rangle_1 \otimes |0\rangle_2. \end{cases}$$

  where

$$|j_1 j_2 jm\rangle = |jm\rangle = \sum_{m_1 m_2} |j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j_2 m_2|jm\rangle = \sum_{m_1+m_2=m} \underbrace{C^j_{m_1 m_2}}_{\substack{\text{C-G} \\ \text{coefficient}}} |m_1 m_2\rangle.$$

  Condon-Shortley phase convention: C-G coefficient $C^j_{m_1 m_2} \in \mathbb{R}, > 0$.
  Clebsch-Gordan coefficients can be found from the table.

Steps to find C-G coefficients $\langle j_1 m_1 j_2 m_2|jm\rangle = C^j_{m_1 m_2}$:

1) find the value of j_1, j_2 from the table;

2) $m_1, m_2 \ \rightarrow$ row of the table;

3) $j, m \ \rightarrow$ column of the table;

4) $-x \ \rightarrow \ -\sqrt{x}$, $x \ \rightarrow \ \sqrt{x}$.

1/2×1/2	1			
	+1	1	0	
+1/2 +1/2	1	0	0	
+1/2 −1/2		1/2	1/2	1
−1/2 +1/2		1/2	−1/2	−1
		−1/2	−1/2	1

Fig. 1: Table of C-G coefficients for $\frac{1}{2} \times \frac{1}{2}$ coupling.

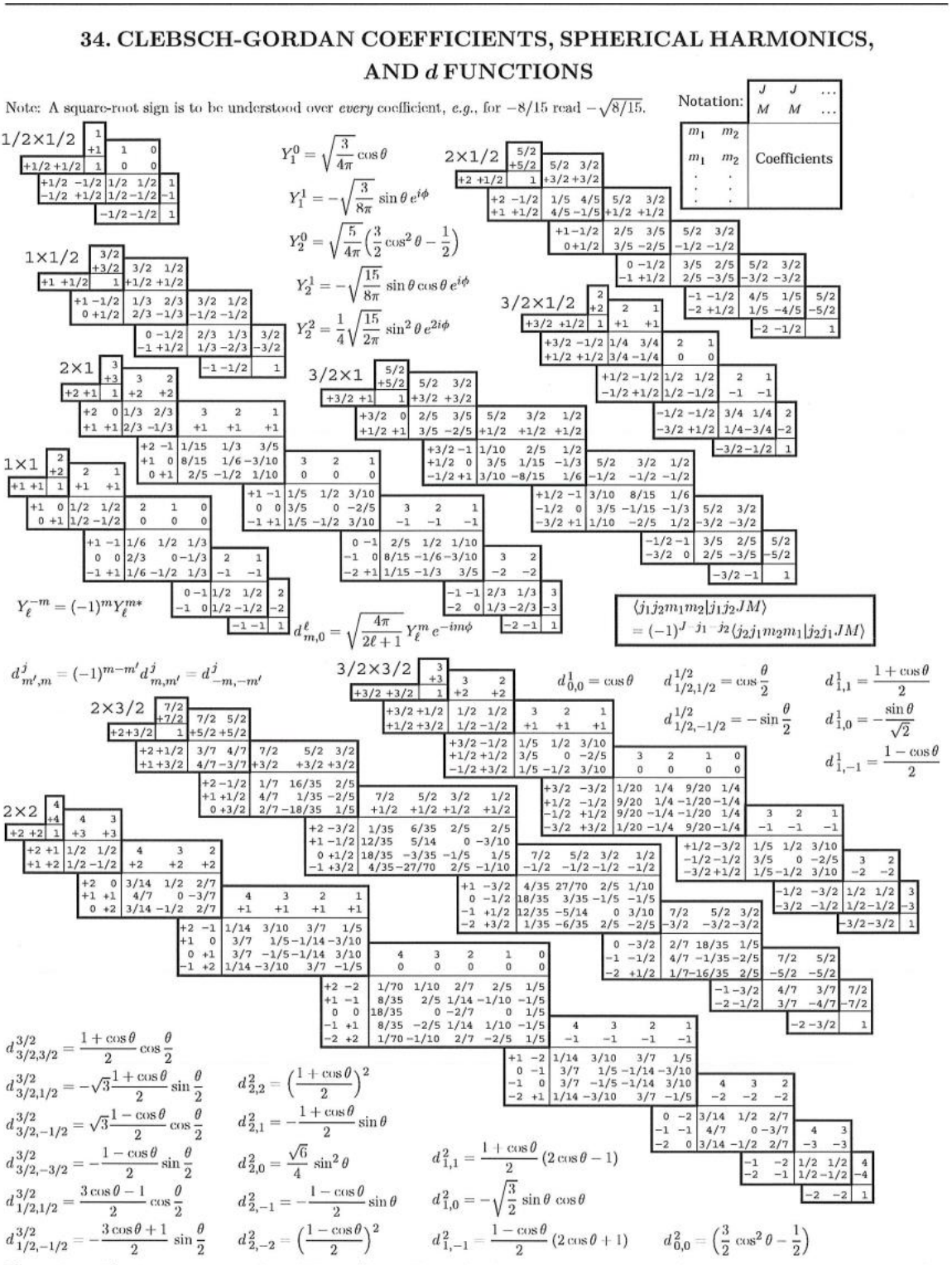


Figure 34.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York. 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York. 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley. New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.

Fig. 2: Table of C-G coefficients.

Properties of C-G coefficients :

a) Real:

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle = \langle j_1 j_2 j m | j_1 j_2 m_1 m_2\rangle = C^{j}_{m_1 m_2} = C^{j*}_{m_1 m_2}.$$

b) Unitarity:

$$\begin{cases} \sum\limits_{m_1,m_2} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j' m'\rangle = \delta_{jj'}\delta_{mm'}; \\ \sum\limits_{m_1,m_2} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle \langle j_1 j_2 m_1' m_2' | j_1 j_2 j m\rangle = \delta_{m_1 m_1'}\delta_{m_2 m_2'}. \end{cases}$$

Basis of AM addition

From the fundamental commutation relations of AM, we have:

$$\left[\hat{J}_i, \hat{J}_j\right] = i\hbar\varepsilon_{ijk}\hat{J}_k \Rightarrow \left[\hat{\boldsymbol{J}}^2, \hat{J}_i\right] \equiv 0.$$

$$\Rightarrow \begin{cases} \hat{\boldsymbol{J}}^2|jm\rangle = j(j+1)\hbar^2|jm\rangle, & (j = 0, 1/2, 1, 3/2, 2, \ldots) \\ \hat{J}_z|jm\rangle = m\hbar|jm\rangle. & (m = \underbrace{-j, -j+1, \ldots, j-1, j}_{(2j+1)\text{-fold}}) \end{cases}$$

Now suppose that we have two AM $\hat{\boldsymbol{J}}_1$, $\hat{\boldsymbol{J}}_2$ satisfying**:**

(1) $\left[\hat{\boldsymbol{J}}_1^2, \hat{J}_{1i}\right] \equiv 0.$

$$\Rightarrow \begin{cases} \hat{\boldsymbol{J}}_1^2|j_1 m_1\rangle = j_1(j_1+1)\hbar^2|j_1 m_1\rangle, \\ \hat{J}_{1z}|j_1 m_1\rangle = m_1\hbar|j_1 m_1\rangle. \end{cases} (m_1 = \underbrace{-j_1, -j_1+1, \ldots, j_1-1, j}_{(2j_1+1)\text{-fold}})$$

(2) $\left[\hat{\boldsymbol{J}}_2^2, \hat{J}_{2i}\right] \equiv 0.$

$$\Rightarrow \begin{cases} \hat{\boldsymbol{J}}_2^2|j_2 m_2\rangle = j_2(j_2+1)\hbar^2|j_2 m_2\rangle, \\ \hat{J}_{2z}|j_2 m_2\rangle = m_2\hbar|j_2 m_2\rangle. \end{cases} (m_2 = \underbrace{-j_2, -j_2+1, \ldots, j_2-1, j}_{(2j_2+1)\text{-fold}})$$

(3) $\hat{\boldsymbol{J}} = \hat{\boldsymbol{J}}_1 + \hat{\boldsymbol{J}}_2 \Rightarrow \left[\hat{J}_{1i}, \hat{J}_{2j}\right] = 0.$

$$\left[\hat{J}_i, \hat{J}_j\right] = \left[\hat{J}_{1i} + \hat{J}_{2i}, \hat{J}_{1j} + \hat{J}_{2j}\right] = i\hbar\varepsilon_{ijk}\hat{J}_k.$$

$$\Rightarrow \left[\hat{\boldsymbol{J}}^2, \hat{J}_i\right] \equiv 0. \Rightarrow \begin{cases} \hat{\boldsymbol{J}}^2|jm\rangle = j(j+1)\hbar^2|jm\rangle, \\ \hat{J}_z|jm\rangle = m\hbar|jm\rangle. \end{cases}$$

but

$$\left[\hat{\boldsymbol{J}}^2, \hat{J}_{1i}\right] = \left[\hat{\boldsymbol{J}}_1^2 + \hat{\boldsymbol{J}}_2^2 + 2\boldsymbol{J}_1 \cdot \hat{\boldsymbol{J}}_2, \hat{J}_{1i}\right] = 2\left[\hat{J}_{1j}, \hat{J}_{1i}\right]\hat{J}_{2j} \neq 0.$$

also, $\left[\hat{\boldsymbol{J}}^2, \hat{J}_{2i}\right] \neq 0$.

(4)

$$\left[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{J}}_1^2\right] = \left[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{J}}_2^2\right] \equiv 0,$$
$$\left[\hat{J}_a, \hat{J}_{1a}\right] = \left[\hat{J}_{1a}, \hat{J}_{1a}\right] + \left[\hat{J}_{2a}, \hat{J}_{1a}\right] \equiv 0.$$

Remark: Relations of CSCO and good quantum numbers. CSCO $(\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{J}}_1^2, \hat{\boldsymbol{J}}_2^2, \hat{J}_z) \Longleftrightarrow$ basis of total/each/magnetic quantum numbers $|j, j_1, j_2, m\rangle$; Observables $(\hat{J}_{1z}, \hat{J}_{2z}, \hat{J}_z) \Longleftrightarrow$ magnetic quantum numbers (m_1, m_2, m).

Two representations (basis)

non-coupling representations (basis):

$$|j_1 m_1\rangle \otimes |j_2 m_2\rangle = |j_1 m_1 j_2 m_2\rangle.$$

$$\sum_{m_1=-j_1}^{j_1} |j_1 m_1\rangle\langle j_1 m_1| = \mathbb{1}; \quad \langle j_1 m_1|j_1 m_1'\rangle = \delta_{m_1 m_1'}.$$
$$\sum_{m_2=-j_2}^{j_2} |j_2 m_2\rangle\langle j_2 m_2| = \mathbb{1}; \quad \langle j_2 m_2|j_2 m_2'\rangle = \delta_{m_2 m_2'}.$$

$$\Rightarrow \begin{cases} \displaystyle\sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2} |j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j_2 m_2| = \mathbb{1}, \\ \displaystyle\sum_{m_1,m_2} |j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j_2 m_2| = \mathbb{1}, \\ \langle j_1 m_1 j_2 m_2|j_1 m_1' j_2 m_2'\rangle = \delta_{m_1 m_1'}\delta_{m_2 m_2'}. \end{cases}$$

Coupling representations (basis):

We can represent states with coupling basis: $|j_1 j_2 j m\rangle$, where the range of j and m are, respectively:

$$j_1 \leqslant m_1 \leqslant j_1; \quad -j_2 \leqslant m_2 \leqslant j_2; \quad -j \leqslant m \leqslant j.$$

Hence, one has

$$-j_1 \leqslant m - m_2 \leqslant j_1; \quad -j_2 \leqslant m - m_1 \leqslant j_2.$$

Let $m = j, m_1 = j_1, m_2 = j_2$, i.e., maximum value for each magnetic quantum numbers, we have:

$$\Rightarrow \begin{cases} -j_1 \leqslant j - j_2 \leqslant j_1 \Rightarrow j_2 - j_1 \leqslant j \leqslant j_1 + j_2, \\ -j_2 \leqslant j - j_1 \leqslant j_2 \Rightarrow j_1 - j_2 \leqslant j \leqslant j_1 + j_2. \end{cases}$$

Then one yields,

$$|j_1 - j_2| \leqslant j \leqslant j_1 + j_2.$$

Exercises:

1*. How to represent the addition of three AM? ($6j$-symbols).

2. Try to represent the coupling of AM by graphic method.

3. Using the table of C-G coefficients, derive the following AM additions: (1) $\frac{1}{2} \times \frac{1}{2}$; (2) $\frac{1}{2} \times 1$; (3) 1×1.

4. Derive the relation of j with j_1 and j_2 in two angular momentum addition.

5. Prove that $m = m_1 + m_2$ for two angular momentum addition.

Lecture Notes 12 Uncertainty Principle

Contents

- Heisenberg's Uncertainty Principle and Generalized Uncertainty Principle;
- Proof of Generalized Uncertainty Principle;
- Minimum Uncertainty State;
- Energy-Time Uncertainty.

Heisenberg's Uncertainty Principle and Generalized Uncertainty Principle (HUP & GUP)

- HUP: $\forall |\psi\rangle$, for $\hat{x}$ and $\hat{p}$, which do not commute, i.e., $[\hat{x}, \hat{p}] = i\hbar$, one has

$$\boxed{\Delta\hat{x} \cdot \Delta\hat{p} \geqslant \frac{\hbar}{2},}$$

  where $\hbar/2$ is called Hesienberg's limit/quantum limit.

- GUP: $\forall |\psi\rangle$, for any two observables $\hat{A}$ and $\hat{B}$, i.e., $[\hat{A}, \hat{B}] \neq 0$, one has

$$\boxed{\Delta\hat{A} \cdot \Delta\hat{B} \geqslant \frac{1}{2}\big|\langle[\hat{A}, \hat{B}]\rangle\big|.}$$

Definition: (mean square deviation/ root mean square deviation)

$$\Delta\hat{A} = \sqrt{\Delta\hat{A}^2} = \sqrt{\big\langle(\hat{A} - \langle\hat{A}\rangle)^2\big\rangle} = \sqrt{\big\langle\hat{A}^2 - \langle\hat{A}\rangle^2\big\rangle},$$
$$\Delta\hat{B} = \sqrt{\Delta\hat{B}^2} = \sqrt{\big\langle(\hat{B} - \langle\hat{B}\rangle)^2\big\rangle} = \sqrt{\big\langle\hat{B}^2 - \langle\hat{B}\rangle^2\big\rangle}.$$

where $\langle\hat{O}\rangle_\psi = \langle\psi|\,\hat{O}\,|\psi\rangle$ (Expectation Value of $\hat{O}$), and $|\psi\rangle$ is normalized.

Proof of Generalized Uncertainty Principle

Define "deviation operator":

$$\hat{\sigma}_A = \hat{A} - \langle\hat{A}\rangle,$$
$$\hat{\sigma}_B = \hat{B} - \langle\hat{B}\rangle.$$

- Properties of $\hat{\sigma}_A, \hat{\sigma}_B$:

$$\begin{cases} \hat{\sigma}_A^\dagger = \hat{\sigma}_A,\ \hat{\sigma}_B^\dagger = \hat{\sigma}_B;\ \text{(hermicity)} \\ \hat{\sigma}_A^\dagger \hat{\sigma}_A = \hat{\sigma}_A^2,\ \hat{\sigma}_B^\dagger \hat{\sigma}_B = \hat{\sigma}_B^2. \end{cases}$$

$$\begin{cases} [\hat{\sigma}_A, \hat{\sigma}_B] = \left[\hat{A}, \hat{B}\right]; \\ [\hat{\sigma}_A, \hat{\sigma}_B]^\dagger = -\left[\hat{\sigma}_A, \hat{\sigma}_B\right];\ \text{(skew-hermitian)} \\ \{\hat{\sigma}_A, \hat{\sigma}_B\}^\dagger = [\hat{\sigma}_A, \hat{\sigma}_B].\ \text{(hermitian)} \end{cases}$$

$$\boxed{\hat{\sigma}_A \hat{\sigma}_B = \frac{1}{2}[\hat{\sigma}_A, \hat{\sigma}_B] + \frac{1}{2}\{\hat{\sigma}_A, \hat{\sigma}_B\}.}$$

$\langle[\hat{\sigma}_A, \hat{\sigma}_B]\rangle$ is purely imaginary, $\langle\{\hat{\sigma}_A, \hat{\sigma}_B\}\rangle$ is purely real. So we have

$$|\langle\hat{\sigma}_A\hat{\sigma}_B\rangle| = \frac{1}{2}|\langle[\hat{\sigma}_A, \hat{\sigma}_B]\rangle + \langle\{\hat{\sigma}_A, \hat{\sigma}_B\}\rangle| \geqslant \frac{1}{2}|\langle[\hat{\sigma}_A, \hat{\sigma}_B]\rangle| = \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle|.$$

Next, we want to prove

$$\boxed{\langle\hat{\sigma}_A^2\rangle\langle\hat{\sigma}_B^2\rangle \geqslant \frac{1}{4}|\langle\hat{\sigma}_A\hat{\sigma}_B\rangle|^2.}$$

From the definition, we know

$$\Delta\hat{A} = \sqrt{\langle\hat{\sigma}_A^2\rangle} = \sqrt{\langle\psi|\,\hat{\sigma}_A^\dagger\hat{\sigma}_A\,|\psi\rangle} = \sqrt{\langle\psi_A|\psi_A\rangle},$$
$$\Delta\hat{B} = \sqrt{\langle\hat{\sigma}_B^2\rangle} = \sqrt{\langle\psi|\,\hat{\sigma}_B^\dagger\hat{\sigma}_B\,|\psi\rangle} = \sqrt{\langle\psi_B|\psi_B\rangle},$$

where $|\psi_{A,B}\rangle = \hat{\sigma}_{A,B}|\psi\rangle$.

From Cauchy-Schwartz inequality, one has

$$\boxed{\langle\psi|\psi\rangle\,\langle\phi|\phi\rangle \geqslant |\,\langle\psi|\phi\rangle\,|^2, \quad \text{equality iff } |\psi\rangle \sim |\phi\rangle\,,}$$

one gets

$$\langle\psi_A|\psi_A\rangle\,\langle\psi_B|\psi_B\rangle \geqslant |\,\langle\psi_A|\psi_B\rangle\,|^2.$$

So

$$\Delta\hat{A}\cdot\Delta\hat{B} \geqslant |\,\langle\psi|\,\hat{\sigma}_A\hat{\sigma}_B\,|\psi\rangle\,|,$$

Note that

$$[\hat{\sigma}_A, \hat{\sigma}_B] = [\hat{A} - \langle\hat{A}\rangle, \hat{B} - \langle\hat{B}\rangle] = [\hat{A}, \hat{B}].$$

So

$$|\langle\psi|\hat{\sigma}_A\hat{\sigma}_B|\psi\rangle| = |\langle\hat{\sigma}_A\hat{\sigma}_B\rangle| \geq \frac{1}{2}|\langle[\hat{\sigma}_A,\hat{\sigma}_B]\rangle| = \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|,$$

which yields GUP

$$\boxed{\Delta\hat{A}\cdot\Delta\hat{B} \geqslant \frac{1}{2}\big|[\hat{A},\hat{B}]\big|.}$$

Let $\hat{A}=\hat{x}$, $\hat{B}=\hat{p}$, then $[\hat{A},\hat{B}]=i\hbar$, one gets Heisenberg's uncertainty principle (HUP):

$$\boxed{\Delta\hat{x}\cdot\Delta\hat{p} \geqslant \frac{\hbar}{2}.}$$

- Review of Cauchy-Schwartz inequality

  Triangle inequality:

$$|\boldsymbol{u}|+|\boldsymbol{v}| \geqslant |\boldsymbol{u}+\boldsymbol{v}| \Rightarrow \boldsymbol{u}^2+\boldsymbol{v}^2+2|\boldsymbol{u}||\boldsymbol{v}| \geqslant \boldsymbol{u}^2+\boldsymbol{v}^2+2\boldsymbol{u}\cdot\boldsymbol{v}.$$

So

$$|\boldsymbol{u}||\boldsymbol{v}| \geqslant \boldsymbol{u}\cdot\boldsymbol{v} = |\boldsymbol{u}||\boldsymbol{v}|\cos\theta, \quad \text{equality iff } \cos\theta = 1,$$

Which yields Cauchy-Schwartz inequality

$$|\boldsymbol{u}|^2|\boldsymbol{v}|^2 \geqslant (\boldsymbol{u}\cdot\boldsymbol{v})^2.$$

Replace $\boldsymbol{u}$ by $|\psi\rangle$, $\boldsymbol{v}$ by $|\phi\rangle$, yields

$$\boxed{\langle\psi|\psi\rangle\langle\phi|\phi\rangle \geqslant |\langle\psi|\phi\rangle|^2, \quad \text{equality iff } |\psi\rangle \sim |\phi\rangle,}$$

Another proof is the follows. Let

$$\boldsymbol{w} = \boldsymbol{u} - \lambda\boldsymbol{v},$$

and since

$$\boldsymbol{w}^2 \geqslant 0,$$

so,

$$(\boldsymbol{u}-\lambda\boldsymbol{v})^2 \geqslant 0,$$

which yields

$$\boxed{|\boldsymbol{u}|^2|\boldsymbol{v}|^2 \geqslant |\boldsymbol{u}\cdot\boldsymbol{v}|^2.}$$

The above inequality can get the equality iff

$$\boxed{\boldsymbol{w}=\boldsymbol{u}-\frac{\boldsymbol{u}\cdot\boldsymbol{v}}{\boldsymbol{v}\cdot\boldsymbol{v}}\boldsymbol{v}\equiv 0\Rightarrow\begin{cases}\boldsymbol{u}\ /\!/\ \boldsymbol{v},\\ \cos\theta=1.\end{cases}}$$

Minimum Uncertainty State (MUS)

Definition: $\exists\,|\psi\rangle$, s.t.

$$\boxed{\Delta\hat{A}\cdot\Delta\hat{B}=\frac{1}{2}\left\langle[\hat{A},\hat{B}]\right\rangle.}$$

This state is called the minimum uncertainty state (MUS).

Remark:

1. $[\hat{A},\hat{B}]\neq 0,\ \forall\,|\psi\rangle\Rightarrow$ GUP.

2. $\forall\hat{A},\ \hat{B},\ [\hat{A},\hat{B}]\neq 0\ ,\exists$ MUS $|\psi\rangle\Rightarrow$ Minimum Uncertainty Relation.

For $\hat{x},\hat{p},\exists$ MUS $|\psi\rangle$, s.t.

$$\Delta\hat{x}\Delta\hat{p}=\frac{\hbar}{2}.$$

Define the deviation operators:

$$\begin{aligned}&\hat{\sigma}_x=\hat{x}-\langle\hat{x}\rangle,\quad \hat{\sigma}_p=\hat{p}-\langle\hat{p}\rangle,\\ &\hat{\sigma}_x^\dagger=\hat{\sigma}_x,\ \hat{\sigma}_p^\dagger=\hat{\sigma}_p,\quad\text{(Hermitian)}\\ &[\hat{\sigma}_x,\hat{\sigma}_p]=i\hbar.\end{aligned}$$

$$\boxed{|\phi\rangle=(\hat{\sigma}_x+i\lambda\hat{\sigma}_p)\,|\psi\rangle\,.}\quad(\lambda\in\mathbb{R})$$

One gets

$$\begin{aligned}\langle\phi|\phi\rangle&=\langle\psi|\,(\hat{\sigma}_x-i\lambda\hat{\sigma}_p)(\hat{\sigma}_x+i\lambda\hat{\sigma}_p)\,|\psi\rangle\\ &=\left\langle\psi\left|\hat{\sigma}_x^2\right|\psi\right\rangle+i\lambda\left\langle\psi\left|[\hat{\sigma}_x,\hat{\sigma}_p]\right|\psi\right\rangle+\lambda^2\left\langle\psi\left|\hat{\sigma}_p^2\right|\psi\right\rangle\\ &=\left\langle\hat{\sigma}_x^2\right\rangle-\lambda\hbar+\lambda^2\left\langle\hat{\sigma}_p^2\right\rangle\geqslant 0,\end{aligned}$$

where

$$\langle\phi|\phi\rangle\geqslant 0,\quad\text{equality iff }|\phi\rangle=\mathbf{0}.$$

Recall that

$$f(x)=ax^2+bx+c,\quad(a>0).$$

one has

$$\Delta = b^2 - 4ac \begin{cases} \leqslant 0 \to f(x) \geqslant 0, \\ = 0 \to f(x) = 0. \end{cases}$$

Note that $a = \langle \hat{\sigma}_p^2 \rangle,\ b = -\hbar,\ c = \langle \hat{\sigma}^2 \rangle$, so

$$(-\hbar)^2 - 4 \left\langle \hat{\sigma}_x^2 \right\rangle \left\langle \hat{\sigma}_p^2 \right\rangle \leqslant 0 \Rightarrow \left\langle \hat{\sigma}_x^2 \right\rangle \left\langle \hat{\sigma}_p^2 \right\rangle \geqslant \frac{\hbar^2}{4},$$

which yields

$$\Delta\hat{x} \cdot \Delta\hat{p} \geqslant \frac{\hbar}{2}. \quad (\Delta\hat{x} = \sqrt{\langle \hat{\sigma}_x^2 \rangle},\ \Delta\hat{p} = \sqrt{\langle \hat{\sigma}_p^2 \rangle}.)$$

When equality?

$$\Delta = b^2 - 4ac = 0 \Longrightarrow \begin{cases} \left\langle \hat{\sigma}_x^2 \right\rangle \left\langle \hat{\sigma}_p^2 \right\rangle = \dfrac{\hbar^2}{4}, \text{ or} \\ \Delta\hat{x} \cdot \Delta\hat{p} = \dfrac{\hbar}{2}. \end{cases}$$

and

$$\lambda = \frac{-b \pm \Delta}{2a} = -\frac{b}{2a} = \frac{\hbar}{2 \left\langle \hat{\sigma}_p^2 \right\rangle}.$$

Since

$$\left\langle \hat{\sigma}_x^2 \right\rangle \left\langle \hat{\sigma}_p^2 \right\rangle = \frac{\hbar^2}{4} \Longrightarrow \left\langle \hat{\sigma}_p^2 \right\rangle = \frac{\hbar^2}{4} \frac{1}{\left\langle \hat{\sigma}_x^2 \right\rangle},$$

one has

$$\lambda = \frac{\hbar}{2} \frac{4 \left\langle \hat{\sigma}_x^2 \right\rangle}{\hbar^2} = \frac{2 \left\langle \hat{\sigma}_x^2 \right\rangle}{\hbar} = \frac{2 \left\langle \Delta x^2 \right\rangle}{\hbar}.$$

When equality holds, $|\psi\rangle \equiv \mathbf{0}$. So

$$\left(\hat{\sigma}_x + i\lambda\hat{\sigma}_p\right) |\psi\rangle = 0,$$

which yields

$$\langle x| \left(\hat{x} - \langle \hat{x} \rangle\right) + i\lambda(\hat{p} - \langle \hat{p} \rangle) |\psi\rangle = 0.$$

Since

$$\begin{cases} \langle x| \left(\hat{x} - \langle \hat{x} \rangle\right) |\psi\rangle = (x - \langle \hat{x} \rangle)\psi(x), \\ \langle x| \, i\lambda(\hat{p} - \langle \hat{p} \rangle) |\psi\rangle = i\lambda \langle x| \left(-i\hbar \dfrac{\mathrm{d}}{\mathrm{d}x}\right) \psi(x) - \langle \hat{p} \rangle |\psi\rangle = \lambda\hbar \dfrac{\mathrm{d}}{\mathrm{d}x}\psi(x) - i\lambda \langle \hat{p} \rangle \psi(x), \end{cases}$$

one has

$$(x - \langle \hat{x} \rangle)\psi(x) - i\lambda \langle \hat{p} \rangle \psi(x) + \lambda\hbar \frac{\mathrm{d}}{\mathrm{d}x}\psi(x) \equiv 0.$$

Assume $\psi(x)$ has the solution as the following,

$$\begin{cases} \psi(x) = e^{i\langle\hat{p}\rangle\cdot x/\hbar} u\left(x - \langle\hat{x}\rangle\right), \\ q = x - \langle\hat{x}\rangle, \end{cases}$$

then equation becomes

$$\left(q + \lambda\hbar\frac{\mathrm{d}}{\mathrm{d}q}\right) u(q) = 0 \Rightarrow \lambda\hbar\frac{\mathrm{d}}{\mathrm{d}q}u = -qu.$$

so

$$\int \frac{\mathrm{d}u(q)}{u(q)} = -\int \frac{q}{\lambda\hbar}\mathrm{d}q \Rightarrow \ln u(q) = -\frac{q^2}{2\lambda\hbar} \Rightarrow u(q) = Ae^{-q^2/2\lambda\hbar},$$

which yields

$$\psi(x) = Ae^{i\langle\hat{p}\rangle x/\hbar} e^{-(x-\langle\hat{x}\rangle)^2/2\lambda\hbar}.$$

Since $\psi(x)$ should be normalized, it follows from Gauss integral:

$$\begin{cases} \int |\psi(x)|^2 \mathrm{d}x = 1, \\ \int_{-\infty}^{+\infty} \mathrm{d}x\ e^{-a(x+b)^2} = \sqrt{\dfrac{\pi}{a}}, \end{cases}$$

then one has

$$\begin{cases} \psi(x) = \left(\dfrac{1}{2\pi\Delta\hat{x}}\right)^{\frac{1}{4}} e^{i\langle\hat{p}\rangle x/\hbar} e^{-\left(\frac{x-\langle\hat{x}\rangle}{2\Delta\hat{x}}\right)^2}, \\ |\psi(x)|^2 = \dfrac{1}{\sqrt{2\pi\Delta\hat{x}}} e^{-2\left(\frac{x-\langle\hat{x}\rangle}{2\Delta\hat{x}}\right)^2}. \end{cases}$$

Two Remarks:

(1) UP always holds, provided that$[\hat{A}, \hat{B}] \neq 0$.
For two conjugate observables, $\hat{A}, \hat{B}$, if $[\hat{A}, \hat{B}] \sim [\hbar]$, then the eigenstate of $\hat{A}$ is the Fourier transfom of the eigenstate of $\hat{B}$.

(2) $\exists\, |\psi\rangle$, which is called the Minimum Uncertaity State (MUS). For two non-commuting observables $\hat{A}$ and $\hat{B}$, i.e., $[\hat{A}, \hat{B}] \neq 0$, one has that in this state, $\Delta\hat{A} \cdot \Delta\hat{B} = \dfrac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle|$ holds. MUS is also called quasi-classical state.

Energy-Time Uncertainty Relation

Energy-time uncertainty relation,

$$\Delta E \cdot \Delta T \geqslant \frac{\hbar}{2}$$

is well-known. However, note that time is NOT an observable! We cannot simply apply the GUP to it.

Consider a system

$$\frac{\partial \hat{H}}{\partial t} \equiv 0.$$

Observable $\hat{A}$

$$\begin{cases} \dfrac{\partial \hat{A}}{\partial t} \equiv 0, \\ [\hat{A}, \hat{H}] \neq 0. \end{cases}$$

Ehrenfest theorem reads:

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \hat{A} \rangle = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle .$$

If

$$[\hat{A}, \hat{H}] \neq 0,$$

then

$$\Delta \hat{A} \cdot \Delta \hat{H} \geqslant \frac{1}{2} \Big| \langle [\hat{A}, \hat{H}] \rangle \Big| = \frac{\hbar}{2} \left| \frac{\mathrm{d}}{\mathrm{d}t} \langle \hat{A} \rangle \right|.$$

So

$$\frac{\Delta \hat{A}}{\left| \mathrm{d} \langle \hat{A} \rangle / \mathrm{d}t \right|} \cdot \Delta \hat{H} \geqslant \frac{\hbar}{2}.$$

Define

$$\Delta T = \frac{\Delta \hat{A}}{\left| \mathrm{d} \langle \hat{A} \rangle / \mathrm{d}t \right|}, \ \Delta H = \Delta E,$$

then one gets

$$\Delta E \cdot \Delta T \geqslant \frac{\hbar}{2}.$$

Exercises:

1. Think about what will happen when we try to determine precisely the position of a particle in a very small region? (Nonrelativity/Relativity)

2. Can you determine all the three components of orbital angular momentum simultaneously? Why?

3. Try to derive the transformation relation of eigenstates of two conjugate observ-

ables.

4. Prove Cauchy-Schwarz inequality.

5. Derive the expression of minimum uncertainty state in position representation.

6. Prove the Generalized Uncertainty Principle (GUP) using Cauchy-Schwartz inequality; also, find out another method to prove GUP.

7. Think about the relations of following:

(1) minimum uncertainty state (wavepacket);

(2) coherent state;

(3) vacuum state;

(4) Gaussian wavepacket.

8. From the condition of MUS, think about the physical significance of MUS.

Lecture Notes 13 Quantum Dynamics

Contents

- Dynamical Equation: Schrödinger's Equation;
- Ehrenfest Theorem;
- Schrödinger's Picture/ Heisenberg's Picture:

Dynamical Equation: Schrödinger's Equation (for a state vector $|\psi(t)\rangle$):

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \;\Rightarrow\; \frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \frac{\hat{H}}{i\hbar}|\psi(t)\rangle.$$

where Hamiltonian $\hat{H}$ is:

$$\hat{H} = \hat{T}(\hat{\boldsymbol{p}}) + \hat{V}(\hat{\boldsymbol{x}}) = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{x}}).$$

Note: The kinetic energy part is $\hat{\boldsymbol{p}}$-dependent only while the potential part is $\hat{\boldsymbol{x}}$-dependent only.

In $\hat{\boldsymbol{x}}-$representation, Schrödigner's equation is:

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t).$$

The equation becomes a partial differential equation (PDE) for the wavefunction $\psi(\boldsymbol{x},t)$ in $\hat{\boldsymbol{x}}$-representation.

• Properties of Schrödinger's equation (SE):

1. SE is an equation of initial value problem (IVP).

$$\text{PDE}\begin{cases}\text{IVP: Initial Value Problem}\\ \text{BVP: Boundary Value Problem}\end{cases}$$

So,

$$\begin{cases}\dfrac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle. & \text{(SE)}\\ |\psi(t=t_0)\rangle = |\psi(t_0)\rangle. & \text{(Initial Value)}\end{cases}$$

2. General expression of SE solution:

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle,$$

where $\hat{U}(t,t_0)$ is the time evolution operator.

When the system is conservative, i.e., $\dfrac{\partial \hat{H}}{\partial t} \equiv 0$, then

$$\hat{U}(t,t_0) = \exp\left[-\frac{i}{\hbar}\hat{H}(t-t_0)\right].$$

Several properties of $\hat{U}(t,t_0)$: Unitary Operator

a. Unitarity:

$$\hat{U}^\dagger = \hat{U}(t_0,t) = \hat{U}^{-1}(t,t_0);\ \hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = \mathbb{1}.$$

b. Chains rule:

$$\hat{U}(t,t_1)\hat{U}(t_1,t_0) = \hat{U}(t,t_0);\ \hat{U}(t,t_n)\hat{U}(t_n,t_{n-1})\cdots\hat{U}(t_1,t_0) = \hat{U}(t,t_0).$$

3. Continuity equation from SE ($\boldsymbol{x}$-representation):

$$\begin{cases} \dfrac{\partial}{\partial t}\psi(\boldsymbol{x},t) = -\dfrac{\hbar}{2mi}\nabla^2\psi(\boldsymbol{x},t) + \dfrac{1}{i\hbar}V(\boldsymbol{x})\psi(\boldsymbol{x},t), \\ \dfrac{\partial}{\partial t}\psi^*(\boldsymbol{x},t) = +\dfrac{\hbar}{2mi}\nabla^2\psi^*(\boldsymbol{x},t) - \dfrac{1}{i\hbar}V(\boldsymbol{x})\psi^*(\boldsymbol{x},t), \end{cases}$$

where $V(\boldsymbol{x}) = V^*(\boldsymbol{x})$ has been assumed. Then one yields:

$$\psi^*\frac{\partial}{\partial t}\psi + \psi\frac{\partial}{\partial t}\psi^* = -\frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*),$$

then

$$\frac{\partial}{\partial t}(\psi^*\psi) + \nabla\cdot\left[\frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)\right] \equiv 0.$$

Let

$$\begin{cases} \rho = \psi^*(\boldsymbol{x},t)\psi(\boldsymbol{x},t), & \text{(probability density)} \\ \boldsymbol{j} = \dfrac{\hbar}{2mi}\big(\psi^*(\boldsymbol{x},t)\nabla\psi(\boldsymbol{x},t) - \psi(\boldsymbol{x},t)\nabla\psi^*(\boldsymbol{x},t)\big). & \text{(probability current density)} \end{cases}$$

$$\Rightarrow\ \frac{\partial}{\partial t}\rho + \nabla\cdot\boldsymbol{j} \equiv 0.$$

4. Ehrenfest's theorem:

$$\text{SE: } \begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \Big(\dfrac{\hat{H}}{i\hbar}\Big)|\psi(t)\rangle; \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)| = \langle\psi(t)|\Big(\dfrac{\hat{H}}{-i\hbar}\Big). \end{cases}$$

So, for $\forall \hat{A}$ one has: $\Big[|\psi(t)\text{ is assumed to be normalized.}\Big]$

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle(t) = \frac{\mathrm{d}}{\mathrm{d}t}\Big(\langle\psi(t)|\hat{A}|\psi(t)\rangle\Big) \\ =&\Big(\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\Big)\hat{A}|\psi(t)\rangle + \Big\langle\psi(t)\Big|\frac{\partial\hat{A}}{\partial t}\Big|\psi(t)\Big\rangle + \langle\psi(t)|\hat{A}\Big(\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle\Big) \\ =&\Big\langle\psi(t)\Big|\Big[-\frac{1}{i\hbar}\hat{H}\hat{A} + \frac{\partial\hat{A}}{\partial t} + \frac{1}{i\hbar}\hat{A}\hat{H}\Big]\Big|\psi(t)\Big\rangle \\ =&\Big\langle\frac{\partial\hat{A}}{\partial t}\Big\rangle(t) + \frac{1}{i\hbar}\Big\langle[\hat{A},\hat{H}]\Big\rangle(t). \end{aligned}$$

Ehrenfest Theorem:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle = \Big\langle\frac{\partial\hat{A}}{\partial t}\Big\rangle + \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle.$$

a) If $\dfrac{\partial\hat{A}}{\partial t} \equiv 0$ (not explicitly dependent on time) and $[\hat{A},\hat{H}] = 0$, then for $\forall\ |\psi(t)\rangle$, $\dfrac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle \equiv 0$ always holds.

b) Conserved quantity (constant of motion) $\hat{A} \Leftrightarrow\ [\hat{A},\hat{H}] \equiv 0$.

c) Comparison of conservation in QM and CM:

$$\begin{cases} \text{CM: If } \dfrac{\partial A}{\partial t} = 0,\ \text{and} [A,H]_{\mathrm{PB}} = 0\ \Rightarrow\ \dfrac{\mathrm{d}}{\mathrm{d}t}A \equiv 0 \Leftarrow\ \dfrac{\mathrm{d}}{\mathrm{d}t}A = \dfrac{\partial A}{\partial t} + [A,H]_{\mathrm{PB}}. \\ \text{QM: If } \dfrac{\partial\hat{A}}{\partial t} = 0,\ \text{and} [\hat{A},\hat{H}] \equiv 0 \Rightarrow\ \dfrac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle \equiv 0 \Leftarrow\ \dfrac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle = \Big\langle\dfrac{\partial\hat{A}}{\partial t}\Big\rangle + \dfrac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle. \end{cases}$$

Note: (1) observable vs expectation value of observable; (2) CCC vs QCC.

Consider $\hat{x}$ and $\hat{p}$ as an example in QM:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\langle\hat{x}\rangle = \dfrac{1}{i\hbar}\langle[\hat{x},\hat{H}]\rangle = \dfrac{1}{i\hbar}\Big\langle[\hat{x},\dfrac{\hat{p}^2}{2m}]\Big\rangle = \dfrac{1}{i\hbar m}\langle[\hat{x},\hat{p}]\hat{p}\rangle = \dfrac{\langle\hat{p}\rangle}{m}; \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = \dfrac{1}{i\hbar}\langle[\hat{p},\hat{H}]\rangle = \dfrac{1}{i\hbar}\langle[\hat{p},V(\hat{x})]\rangle = \dfrac{1}{i\hbar}\Big\langle[\hat{p},\hat{x}]\dfrac{\partial\hat{V}}{\partial x}\Big\rangle = -\Big\langle\dfrac{\mathrm{d}}{\mathrm{d}x}V(x)\Big\rangle. \end{cases}$$

So,

$$\begin{cases} m\dfrac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\hat{x}\rangle = -\Big\langle\dfrac{\mathrm{d}}{\mathrm{d}x}V(x)\Big\rangle, & \text{(QM)} \\ m\dfrac{\mathrm{d}^2}{\mathrm{d}t^2}x = -\dfrac{\mathrm{d}}{\mathrm{d}x}V(x). & \text{(CM)} \end{cases}$$

That is to compare (in 3 dimensional space)

$$-\langle\nabla V(\boldsymbol{x})\rangle \text{ vs } -\nabla V(\boldsymbol{x}).$$

If $-\langle\nabla V(\boldsymbol{x})\rangle \cong -\nabla V(\boldsymbol{x})$, then QM $\cong$ CM.

Schrödinger's Picture/ Heisenberg's Picture

Schrödinger's Picture:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle_S = \dfrac{1}{i\hbar}\hat{H}_S|\psi(t)\rangle_S; \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\hat{A}_S(t) \equiv 0. \end{cases}$$

Heisenberg's Picture:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle_H \equiv 0, \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\hat{A}_H(t) = \Big(\dfrac{\partial\hat{A}_S(t)}{\partial t}\Big)_H + \dfrac{1}{i\hbar}[\hat{A}_H, \hat{H}_H]. \end{cases}$$

[Proof]:

S.E. $\Rightarrow |\psi(t)\rangle_S = \hat{U}(t)|\psi(t)\rangle_H,\ \hat{U} = e^{-i\hat{H}_S t/\hbar},\ \hat{U}^\dagger = e^{i\hat{H}_S t/\hbar}$.

Then, from ${}_S\langle\psi|\psi\rangle_S =_H \langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle_H \equiv 1,$ it can be shown that $\hat{U}^\dagger(t)\hat{U}(t) = \mathbb{1}$.

$\langle\hat{A}(t)\rangle =_S \langle\psi|\hat{A}_S(t)|\psi\rangle_S =_H \langle\psi|\hat{U}^\dagger\hat{A}_S(t)\hat{U}|\psi\rangle_H \equiv_H \langle\psi|\hat{A}_H|\psi\rangle_H$, so one yields $\hat{A}_H = \hat{U}^\dagger(t)\hat{A}_S\hat{U}(t)$.

So we have:

$$\begin{aligned}
\frac{\mathrm{d}\hat{A}_H}{\mathrm{d}t} &= \frac{\partial\hat{U}^\dagger}{\partial t}\hat{A}_S\hat{U} + \hat{U}^\dagger\Big(\frac{\partial\hat{A}_S}{\partial t}\Big)\hat{U} + \hat{U}^\dagger\hat{A}_S\frac{\partial\hat{U}}{\partial t} \\
&= \frac{i}{\hbar}\Big[\hat{U}^\dagger\hat{H}\hat{A}_S\hat{U} - \hat{U}^\dagger\hat{A}_S\hat{H}\hat{U}\Big] + \Big(\frac{\partial\hat{A}_S}{\partial t}\Big)_H \\
&= \frac{1}{i\hbar}\Big[\hat{U}^\dagger\hat{A}_S\hat{U}\hat{U}^\dagger\hat{H}\hat{U} - \hat{U}^\dagger\hat{H}\hat{U}\hat{U}^\dagger\hat{A}_S\hat{U}\Big] + \Big(\frac{\partial\hat{A}_S}{\partial t}\Big)_H \\
&= \frac{1}{i\hbar}\big[\hat{A}_H\hat{H}_H - \hat{H}_H\hat{A}_H\big] + \Big(\frac{\partial\hat{A}_S}{\partial t}\Big)_H \\
&= \Big(\frac{\partial\hat{A}_S}{\partial t}\Big)_H + \frac{1}{i\hbar}[\hat{A}_H, \hat{H}_H];\ \text{Note that } \boxed{\hat{H}_H = \hat{H}_S.}
\end{aligned}$$

Also,

$$\begin{aligned}
&|\psi(t)\rangle_H = \hat{U}^\dagger|\psi(t)\rangle_S \\
\Rightarrow &\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle_H = \Big(\frac{\partial\hat{U}^\dagger}{\partial t}\Big)|\psi(t)\rangle_S + \hat{U}^\dagger\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle_S \\
&= -\frac{1}{i\hbar}\big[\hat{U}^\dagger\hat{H}_S - \hat{U}^\dagger\hat{H}_S\big]|\psi(t)\rangle_S \equiv 0.
\end{aligned}$$

Exercises:

1. Suppose $V(x) = \sum_n V_n x^n$, prove that for $n = 0, n = 1$, QM $\cong$ CM, while for $n \geq 2$, QM is different from CM.

2. Using the transformation operator, derive the equations of Heisenberg's pictures from Schrödinger's picture, and vice versa.

3. Prove the unitarity and chain's rule for the transformation operator $\hat{U}(t, t_0)$.

4. If $\dfrac{\partial\hat{H}}{\partial t} \neq 0$, derive the expression of $\hat{U}(t, t_0)$.

5. Derive the continuity equation from Schrödinger's equation. Further, consider the case if the potential is not a real function.

6. Derive Ehrenfest's theorem from Schrödinger's equation.

Lecture Notes 14 Symmetry Transformation and Conservation

Contents

- Symmetry Transformation and Conservation;
- Two kinds of Unitary Transformations (Operators);
- Space Translation Transformation;
- Time Translation Transformation;
- Space Rotation Transformation.

1. Symmetry Transformation and Conservation:

Suppose an observable $\hat{A}$ meets the following conditions:

$$\frac{\partial \hat{A}}{\partial t} \equiv 0, \ [\hat{A}, \hat{H}] \equiv 0.$$

From Ehrenfest's theorem:

$$\boxed{\frac{\mathrm{d}\langle \hat{A} \rangle}{\mathrm{d}t} = \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle.}$$

yields

$$\boxed{\frac{\mathrm{d}\langle \hat{A} \rangle}{\mathrm{d}t} \equiv 0.}$$

In the above, $\hat{A}$ is called a constant of motion, corresponding to a conserved quantity.
Symmetry transformation $\hat{U}$: linearity and unitarity.

$$\boxed{\begin{aligned} &\forall\ |\psi\rangle \to |\psi'\rangle = \hat{U}|\psi\rangle, \\ &\quad |\phi\rangle \to |\phi'\rangle = \hat{U}|\phi\rangle. \end{aligned}}$$

Three things are kept invariant:

(1) Inner product of state vectors: $\langle \phi' | \psi' \rangle = \langle \phi | \psi \rangle$.

$$\langle \phi' | \psi' \rangle = \langle \phi | \hat{U}^\dagger \hat{U} \rangle | \psi \rangle = \langle \phi | \psi \rangle.$$

leading to:

$$\boxed{\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \mathbb{1}; \quad \hat{U}^\dagger = \hat{U}^{-1}.}$$

(2) Expectation value of observables: $\langle\hat{A}'\rangle_{\psi'} \equiv \langle\hat{A}\rangle_\psi$

$\forall\ |\psi\rangle$ and $\langle\psi|\psi\rangle = 1$, we have:

$$\begin{cases} \langle\hat{A}'\rangle_{\psi'} = \langle\psi'|\hat{A}'|\psi'\rangle = \langle\psi|\hat{U}^\dagger\hat{A}'\hat{U}|\psi\rangle. \\ \langle\hat{A}\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle. \end{cases}$$

so

$$\boxed{\hat{A} = \hat{U}^\dagger\hat{A}'\hat{U}; \quad \hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger.}$$

(3) Hamiltonian $\hat{H}$: $\hat{H}' \equiv \hat{H}$.

$$\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger = \hat{H} \Longrightarrow \hat{U}\hat{H} = \hat{H}\hat{U} \to \boxed{[\hat{U}, \hat{H}] \equiv 0.}$$

2. Two kinds of Unitary Transformations (Operators)

(1) Discrete Unitary Transformation (Operators):

Unitary+Hermitian+Involutary Operators ⇒ "Trinity" Operator:

$$\boxed{\hat{U}^\dagger = \hat{U}^{-1};\ \hat{U}^\dagger = \hat{U};\ \hat{U}^2 = \mathbb{1}.}$$

(a) Space Reflection/Inversion Operator (Parity):

$$\boxed{\hat{\pi}|\boldsymbol{x}\rangle = |-\boldsymbol{x}\rangle} \to \begin{cases} \hat{\boldsymbol{x}} \xrightarrow{\hat{\pi}} \hat{\boldsymbol{x}}' = \hat{\pi}\hat{\boldsymbol{x}}\hat{\pi}^\dagger = -\hat{\boldsymbol{x}} \leftrightarrow \{\boldsymbol{x}, \hat{\pi}\} = 0, \\ \hat{\boldsymbol{p}} \xrightarrow{\hat{\pi}} \hat{\boldsymbol{p}}' = \hat{\pi}\hat{\boldsymbol{p}}\hat{\pi}^\dagger = -\hat{\boldsymbol{p}} \leftrightarrow \{\boldsymbol{p}, \hat{\pi}\} = 0. \end{cases}$$

If $[\hat{\pi}, \hat{H}] = 0$, then Conservation of Parity holds. $(\hat{\pi}^\dagger = \hat{\pi} = \hat{\pi}^{-1};\ \hat{\pi}^2 = \mathbb{1})$

(b) Transposition Operators（交换算符，置换中的一个特例):

$$\hat{T}_{ij}|\cdots u_i \cdots u_j \cdots\rangle = |\cdots u_j \cdots u_i \cdots\rangle. \to \boxed{\hat{T}_{ij}^\dagger = \hat{T}_{ij} = \hat{T}_{ij}^{-1}.}$$

If $[\hat{T}_{ij}, \hat{H}] = 0$, e.g.,

$$\hat{H} = \frac{\boldsymbol{p}_1^2}{2m} + \frac{\boldsymbol{p}_2^2}{2m} + \frac{1}{|\boldsymbol{x}_1 - \boldsymbol{x}_2|},$$

$$\text{we have } \underline{\text{Conservation of Exchange Symmetry}} \begin{cases} \text{Symmetric} \ \rightarrow \ \text{Bosons.} \\ \text{Anti-symmetric} \ \rightarrow \ \text{Fermions.} \end{cases}$$

(2) Continuous Unitary Transformation (Operators):
Consider an infinitesimal unitary transformations,

(a) $\hat{u}(\epsilon) = \mathbb{1} + i\epsilon\hat{F}$ (Lie algebra)
ϵ : infinitesimal parameter; $\hat{F}$: generator of a Lie group (生成元)

$$\begin{aligned} & \hat{u}\hat{u}^\dagger = \hat{u}^\dagger\hat{u} = \mathbb{1} \\ \Longrightarrow \quad & (\mathbb{1} + i\epsilon\hat{F})(\mathbb{1} - i\epsilon\hat{F}^\dagger) = \mathbb{1} \\ \Longrightarrow \quad & \mathbb{1} + i\epsilon(\hat{F} - \hat{F}^\dagger) + O(\epsilon^2) = \mathbb{1} \\ \Longrightarrow \quad & \boxed{\hat{F}^\dagger = \hat{F}.} \end{aligned}$$

(b) if $\epsilon = a/N$, $(N \gg 1)$

$$\lim_{N\to\infty} \hat{U}(a) = \lim_{N\to\infty} \hat{u}^N(\epsilon) = \lim_{N\to\infty} \left(1 + i\frac{a}{N}\hat{F}\right)^N = e^{ia\hat{F}},$$

$$\Rightarrow \begin{cases} \hat{U}(a) = e^{ia\hat{F}}, \\ \hat{u}(\epsilon) = 1 + i\epsilon\hat{F}. \end{cases} \xrightarrow{\text{Lie Group}} \begin{cases} \hat{F}^\dagger = \hat{F} \text{fi} \\ [\hat{F}, \hat{H}] \equiv 0\Theta \end{cases} \Rightarrow \hat{F} \text{ is a conserved quantity.}$$

3. Space Translation Transformation:

Definition:

$$\begin{aligned} |x'\rangle = & \boxed{\hat{T}(a)|x\rangle = |x + a\rangle} \Rightarrow \langle x|\hat{T}^\dagger(a) = \langle x + a| = \langle x'|. \\ \Longrightarrow \quad & \langle x_1'|x'\rangle = \langle x_1|\hat{T}^\dagger(a)\hat{T}(a)|x\rangle = \langle x_1|x\rangle = \delta(x - x_1). \\ & \langle x_1'|x'\rangle = \langle x_1 + a|x + a\rangle = \delta(x - x_1). \\ \Longrightarrow \quad & \boxed{\begin{cases} \hat{T}^\dagger(a) = \hat{T}^{-1}(a) = \hat{T}(-a), \\ \hat{T}^\dagger(a)\hat{T}(a) = \hat{T}(a)\hat{T}^\dagger(a) = \mathbb{1}. \end{cases}} \end{aligned}$$

Apply Hermitian conjugate to both sides, one has:

$$\begin{aligned} & \hat{T}(-a)|x\rangle = |x - a\rangle \\ \Rightarrow \ & \langle x|\hat{T}^\dagger(-a) = \langle x - a| \\ \Rightarrow \ & \boxed{\langle x|\hat{T}(a) = \langle x - a|.} \end{aligned}$$

Also, calculate the commutation relations

$$\begin{aligned}&[\hat{x}\hat{T}(a)-\hat{T}(a)\hat{x}]|x\rangle=\hat{x}\hat{T}(a)|x\rangle-\hat{T}(a)\hat{x}|x\rangle\\=&\hat{x}|x+a\rangle-x\hat{T}(a)|x\rangle=(x+a)|x+a\rangle-x|x+a\rangle\\=&a|x+a\rangle=a\hat{T}(a)|x\rangle,\end{aligned}$$

which implies that

$$\boxed{[\hat{x},\hat{T}(a)]=a\hat{T}(a).}$$

Then:

$$\begin{aligned}&\hat{x}\hat{T}(a)=\hat{T}(a)\hat{x}+a\hat{T}(a),\\&\hat{x}=\hat{T}(a)\hat{x}\hat{T}^{\dagger}(a)+a,\ \text{or}\ \hat{T}(a)\hat{x}\hat{T}^{\dagger}(a)=\hat{x}-a\mathbb{1},\end{aligned}$$

or

$$\hat{T}^{\dagger}(a)\hat{x}\hat{T}(a)=\hat{x}+a\mathbb{1}.$$

$$\langle x|\hat{T}^{\dagger}(a)\hat{x}\hat{T}(a)|x\rangle=\langle x|(\hat{x}+a)|x\rangle=\langle x+a|\hat{x}|x+a\rangle=x+a.$$

Infinitesimal Translation:

Use the Taylor expansion, one has

$$\hat{T}(a)=\hat{T}(0)+a\frac{\partial\hat{T}}{\partial a}(0)+\cdots.$$

Define an operator:

$$\hat{k}=i\frac{\partial\hat{T}}{\partial a}(0),$$

and consider an infinitesimal transition $\hat{t}(\epsilon)$, one has:

$$\hat{T}(a)=1-ia\hat{k}+\cdots\xrightarrow{a=\epsilon\to0}\hat{t}(\epsilon)=1-i\epsilon\hat{k}.$$

From the definition of differentiation:

$$\frac{\mathrm{d}\hat{T}(a)}{\mathrm{d}a}=\lim_{\epsilon\to0}\frac{\hat{T}(a+\epsilon)-\hat{T}(a)}{\epsilon}=\Big(\lim_{\epsilon\to0}\frac{\hat{t}(\epsilon)-1}{\epsilon}\Big)\hat{T}(a)=-i\hat{k}\hat{T}(a).$$

we have:

$$\boxed{\hat{T}(a)=e^{-ia\hat{k}}.}$$

We can also get this result from the relation between infinitesimal generator and the finite displacement. As

$$\hat{T}(a)=\hat{T}^{N}(\epsilon),\quad\epsilon=a/N,$$

one has:

$$\hat{T}(a) = \lim_{N\to\infty}(1 - i\epsilon\hat{k})^N = \lim_{N\to\infty}(1 - i\frac{a\hat{k}}{N})^N = e^{-ia\hat{k}}.$$

Now let's find the meaning of the operator $\hat{k}$, we have:

$$\hat{k}|x\rangle = i\frac{\partial\hat{T}(a)}{\partial a}|x\rangle\Big|_{a=0} = i\frac{\partial}{\partial a}|x+a\rangle\Big|_{a=0} = i\frac{\partial}{\partial x}|x\rangle.$$

While in x-representation, we have:

$$(\hat{k}\psi)(x) = i\Big(\frac{\partial\hat{T}(a)}{\partial a}\psi\Big)(x) = i\frac{\partial}{\partial a}\psi(x-a)\Big|_{a=0} = -i\frac{\partial}{\partial x}\psi(x).$$

so we get:

$$\hat{k} = -i\frac{\partial}{\partial x}$$

The final step is to use the expression of $\hat{p}$ in x-representations:

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \to \hat{p} = \hbar\hat{k}.$$

In conclusion, we have:

$$\boxed{\begin{cases}\hat{t}(\epsilon) = \mathbb{1} - \dfrac{i}{\hbar}\epsilon\hat{p};\\ \hat{T}(a) = e^{-ia\hat{p}/\hbar}.\end{cases}}$$

If we have $[\hat{T}(a), \hat{H}] = 0$, then $[\hat{p}, \hat{H}] = 0$, i.e., momentum $\hat{p}$ is conserved.

4. Time Translation:

Definition:

$$\hat{U}(\tau)|\psi(t)\rangle = |\psi(t-\tau)\rangle. \begin{cases}\hat{U}(\tau) = e^{i\tau\hat{H}/\hbar}.\\ \hat{u}(\epsilon) = \mathbb{1} + i\epsilon\hat{H}/\hbar.\end{cases}$$

Conservation:

$$[\hat{U}(\tau), \hat{H}] \equiv 0 \longrightarrow \boxed{[\hat{H}, \hat{H}] \equiv 0.} \quad \text{(Energy conservation, provided that } \frac{\partial\hat{H}}{\partial t} = 0.$$

5. (Space) Rotation Transformation

Definition:

$$\begin{cases}\hat{U}(\hat{\boldsymbol{n}}, \theta) = e^{-\frac{i}{\hbar}\theta(\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{L}})},\\ \hat{u}(\hat{\boldsymbol{n}}, \epsilon) = \mathbb{1} - \dfrac{i}{\hbar}\epsilon(\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{L}}).\end{cases}$$

Proof:

Let $\hat{\boldsymbol{n}}$ be the unit verctor parallel to the axis of rotation; after the Space Rotation Transformation, we have:

$$\boldsymbol{x} \to \boldsymbol{x}' = \boldsymbol{x} + \delta\boldsymbol{x} = \boldsymbol{x} + \epsilon(\hat{\boldsymbol{n}} \times \boldsymbol{x}).$$

Use the Translation Transformation, we have:

$$\begin{aligned}\hat{t}(\delta\boldsymbol{x}) &= \mathbb{1} - i\delta\boldsymbol{x} \cdot \hat{\boldsymbol{p}}/\hbar \\ &= \mathbb{1} - i\epsilon(\hat{\boldsymbol{n}} \times \hat{\boldsymbol{x}}) \cdot \hat{\boldsymbol{p}}/\hbar \\ &= \mathbb{1} - i\epsilon\hat{\boldsymbol{n}} \cdot (\hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}})/\hbar \\ &= \mathbb{1} - i\epsilon\hat{n} \cdot \hat{\boldsymbol{L}}/\hbar.\end{aligned}$$

So we have:

$$\hat{u}(\hat{\boldsymbol{n}}, \epsilon) = \hat{t}(\delta\boldsymbol{x}) = \mathbb{1} - \frac{i}{\hbar}\epsilon(\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{L}}),$$

then we have:

$$\hat{U}(\hat{\boldsymbol{n}}, \theta) = e^{-\frac{i}{\hbar}\theta(\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{L}})}.$$

If $[\hat{U}(\hat{\boldsymbol{n}}, \theta), \hat{H}] \equiv 0$, then:

$$[\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{L}}, \hat{H}] = 0 \longrightarrow \boxed{[\hat{\boldsymbol{L}}_n, \hat{H}] \equiv 0.}$$

That is to say, the $\hat{\boldsymbol{n}}$ component of angular momentum is conserved.

Let's discuss the general case of rotation:

$$\begin{cases}\boldsymbol{v} = \boldsymbol{v}_\parallel + \boldsymbol{v}_\perp, \\ \boldsymbol{v}_\parallel = (\boldsymbol{v} \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}}, \\ \boldsymbol{v}_\perp = \boldsymbol{v} - \boldsymbol{v}_\perp = \boldsymbol{v} - (\boldsymbol{v} \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}}.\end{cases} \qquad \begin{cases}\boldsymbol{v}' = \boldsymbol{v}'_\parallel + \boldsymbol{v}'_\perp, \\ \boldsymbol{v}'_\parallel = \boldsymbol{v}_\parallel = (\boldsymbol{v} \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}}, \\ \boldsymbol{v}'_\perp = \boldsymbol{v}_\perp \cos\theta + (\hat{\boldsymbol{n}} \times \boldsymbol{v}) \sin\theta.\end{cases}$$

so we have:

$$\begin{aligned}\boldsymbol{v}' &= \boldsymbol{v}'_\parallel + \boldsymbol{v}'_\perp \\ &= (\boldsymbol{v} \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}} + \boldsymbol{v}_\perp \cos\theta + (\hat{\boldsymbol{n}} \times \boldsymbol{v}) \sin\theta \\ &= (\boldsymbol{v} \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}} + [\boldsymbol{v} - (\boldsymbol{v} \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}}] \cos\theta + (\hat{\boldsymbol{n}} \times \boldsymbol{v}) \sin\theta.\end{aligned}$$

So we get the Roderigures rotation formula:

$$\boxed{\boldsymbol{v}' = \boldsymbol{v} \cos\theta + (1 - \cos\theta)(\boldsymbol{v} \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{n}} + (\hat{\boldsymbol{n}} \times \boldsymbol{v}) \sin\theta.}$$

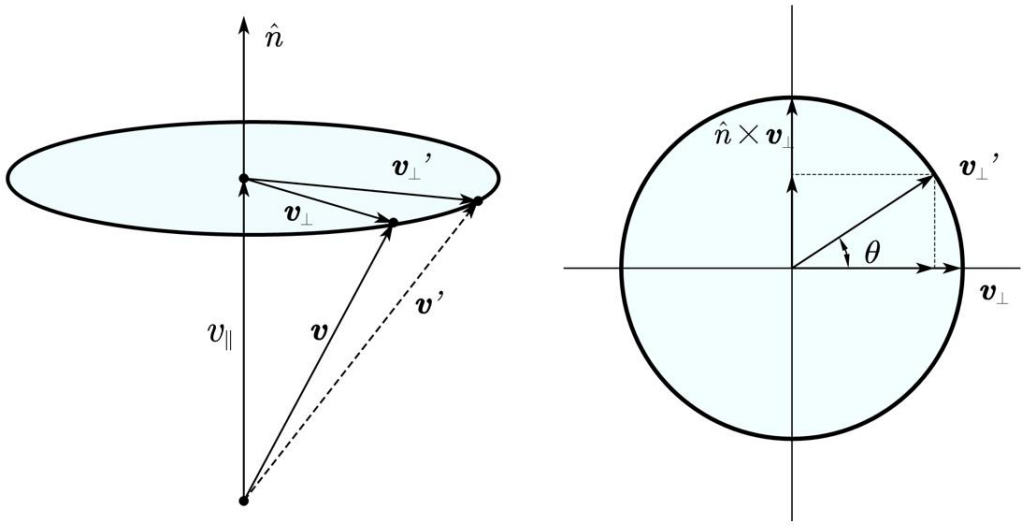


Fig. 3: Rotation Transformation

After rotation, $\boldsymbol{v} \to \boldsymbol{v}'$ (let $\boldsymbol{v} = \boldsymbol{x}$);

$$\boldsymbol{x}' = \boldsymbol{x}\cos\theta + (1-\cos\theta)(\boldsymbol{x}\cdot\hat{\boldsymbol{n}})\hat{\boldsymbol{n}} + (\hat{\boldsymbol{n}}\times\boldsymbol{x})\sin\theta.$$

If $\theta \ll 1$, then $\cos\theta \approx 1 + O(\theta^2),\ \sin\theta \approx \theta + O(\theta^3)$,

$$\boldsymbol{x}' = \boldsymbol{x} + (\hat{\boldsymbol{n}}\times\boldsymbol{x})\theta.$$
$$\to \boxed{\delta\boldsymbol{x} = \boldsymbol{x}' - \boldsymbol{x} = \theta(\hat{\boldsymbol{n}}\times\boldsymbol{x}).}$$

Two Representations of Rotations: $\begin{cases} \hat{R}(\hat{\boldsymbol{n}},\theta): \text{ Axis-Angle Representation (AA-representation)} \\ \hat{R}(\alpha,\beta,\gamma): \text{Euler Angle Representation (EA-representation)} \end{cases}$

Be careful to avoid "Gimbal Lock" （万向锁）!

Exercises:

1. Compare Ehrenfest's theorem with Newton's second law.

2. Derive the following properties of the space translation transformation. You can

start form the definition: $\hat{T}(a)|x\rangle = |x+a\rangle$.

$$\begin{cases} \hat{T}(0) = \mathbb{1}; \\ \hat{T}(a)\hat{T}(b) = \hat{T}(a+b) = \hat{T}(b)\hat{T}(a); \\ \hat{T}^{-1}(a) = \hat{T}(-a); \\ \hat{T}^{-1}(a) = \hat{T}^{\dagger}(a). \end{cases}$$

3. How does the space translation transformation act on the wave function?

4. Prove Roderigures rotation formula.

5. Derive the expression of space translation, time translation and space rotation operators.

6. Prove that the transposition operator is a Hermitian, unitary, and involutory operator.

7. What are the properties of unitary transformations? Why?

Lecture Notes 15 Well Problem

Contents

- Preliminaries;
- 1D Infinite Square Well Problem;
- 1D Finite Square Well.

1. Pereliminaries

1-D Schrödinger's Equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x,t)\psi(x,t).$$

When $\dfrac{\partial \hat{V}(x,t)}{\partial t} = 0$, (s.t. $\dfrac{\partial \hat{H}}{\partial t} \equiv 0$) $\Rightarrow$ Stationary Schrödinger's Equation.

Several Terminologies:

a) Stationary Schrödinger's Equation (SSE);

b) Time-independent Schrödinger's Equation;

c) Energy Eigenvalue Equation.

$$\Big[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\Big]\psi(x) = E\psi(x).$$

Several Typical Problems:

- Well Problem: Infinite Square Well; Finite Square Well $\Rightarrow$ Bound State Problem
- Barrier Problem: Finite (Square) Barrier; Step Barrier Probelm $\Rightarrow$ Unbound State Problem $\Leftrightarrow$ Scattering Problem
- Some General Discussions:

1D Infinite Square Well:

For 1-D Schrödinger's Equation:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right]\psi(x)=E\psi(x),$$

where

$$V(x)=\begin{cases}0, & |x|<a/2,\\ \infty. & |x|\geq a/2.\end{cases}$$

Boundary condition analysis:

$$\begin{cases}1)\ \text{when } |x|>a/2, \psi(x)=0,\ \text{Convergence condition must be satisfied.}\\ \quad\Rightarrow\ \displaystyle\int_{\infty}^{\infty}|\psi(x)|^2\mathrm{d}x<\infty\Rightarrow\ \psi(x)\xrightarrow{x\to\infty}0.\\ 2)\ \text{when } |x|=\pm\dfrac{a}{2},\ \text{continuous function}\Rightarrow\ \psi\Big(\pm\dfrac{a}{2}\Big)=0.\end{cases}$$

Inside square well ($x\in\left[-\frac{a}{2},+\frac{a}{2}\right]$), $V(x)=0\ \Rightarrow\ k^2=\dfrac{2mE}{\hbar^2}$,

$$-\frac{\hbar^2}{2m}\psi(x)=E\psi(x)\ \Rightarrow\ \psi(x)=Ae^{ikx}+Be^{-ikx}.$$

According to the boundary condition 2) $\Rightarrow$ $\psi(\pm\frac{a}{2})=0$ $\Rightarrow$ $e^{2ika}=1$ $\Rightarrow$ $2ka=2n\pi$ $\Rightarrow$ $A=(-)^{n+1}B, (n\in\mathbb{Z})$.

$$\Rightarrow\ E_n=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2}{2m}\cdot\Big(\frac{n\pi}{a}\Big)^2=\frac{\hbar^2\pi^2}{2ma^2}n^2=\varepsilon n^2,$$

where

$$\varepsilon=\frac{\hbar^2\pi^2}{2ma^2}=\frac{\hbar^2}{8ma^2}.\quad\text{(Ground State Energy)}$$

$$\Rightarrow\ \psi(x)=\begin{cases}2A\cos\Big(\dfrac{n\pi x}{a}\Big),\ (|x|<a/2, n=\text{odd})\\ 2A\sin\Big(\dfrac{n\pi x}{a}\Big).\ (|x|<a/2, n=\text{even})\end{cases}$$

Normalization ($\int_{-\infty}^{\infty}|\psi(x)|^2\mathrm{d}x=1$) $\Rightarrow$ $A=\dfrac{1}{a}\in\mathrm{R}$.

$$\Rightarrow\ \psi(x)=\begin{cases}\dfrac{2}{a}\cos\Big(\dfrac{n\pi x}{a}\Big),\ (|x|<a/2, n=\text{odd})\ \Rightarrow\ \text{even parity}\\ \dfrac{2}{a}\sin\Big(\dfrac{n\pi x}{a}\Big).\ (|x|<a/2, n=\text{even})\ \Rightarrow\ \text{odd parity}\end{cases}\Rightarrow\text{explicit parity.}$$

Summary:

- Potential:

$$V(x)=\begin{cases}\infty, & (|x|\geq a/2);\\ 0, & (|x|<a/2).\end{cases}\Rightarrow \text{ even potential } V(-x)=V(x).$$

- Solution: (Bound State $\Rightarrow$ Discrete Solutions)

$$\psi_n(x)=\begin{cases}\dfrac{2}{a}\cos\Big(\dfrac{n\pi}{a}x\Big), & \Big(|x|<\dfrac{a}{2}\Big)\\ \dfrac{2}{a}\sin\Big(\dfrac{n\pi}{a}x\Big), & \Big(|x|<\dfrac{a}{2}\Big)\end{cases}$$

$$E_n=\frac{\hbar^2\pi^2}{2ma^2}n^2=\varepsilon_g\cdot n^2,\ (n=1,2,\cdots\in\mathbb{Z}^+)$$

where

$$\varepsilon_g=\frac{\hbar^2\pi^2}{2ma^2}.$$

is the ground state energy.

- Nodes:

  $\psi_n(x)$ has $(n-1)$ nodes. [No nodes for ground state!]

- Boundary condition:

$$\psi\Big(\frac{a}{2}\Big)=0;\ \psi\Big(-\frac{a}{2}\Big)=0.$$

Two boundary conditions for 2nd-order differential equation.

Since $V(x)=V(-x)$, $\dfrac{\boldsymbol{p}^2}{2m}=\dfrac{(-\boldsymbol{p})^2}{2m}=\dfrac{\Big[\dfrac{\mathrm{d}(-\boldsymbol{x})}{\mathrm{d}t}\Big]^2}{2m}$, both are even function $\Rightarrow$ $\hat{H}$ is an even operator.

Even operator $\Rightarrow$ Even states $\Rightarrow$ Explicit parity of eigenstates of $\hat{H}$.

1D Finite Square Well

- Potential: (even potential, $V(-x)=V(x)$.)

$$V(x)=\begin{cases}-V_0, & (|x|<a)\\ 0, & (|x|\geq a)\end{cases}\qquad (V_0>0).$$

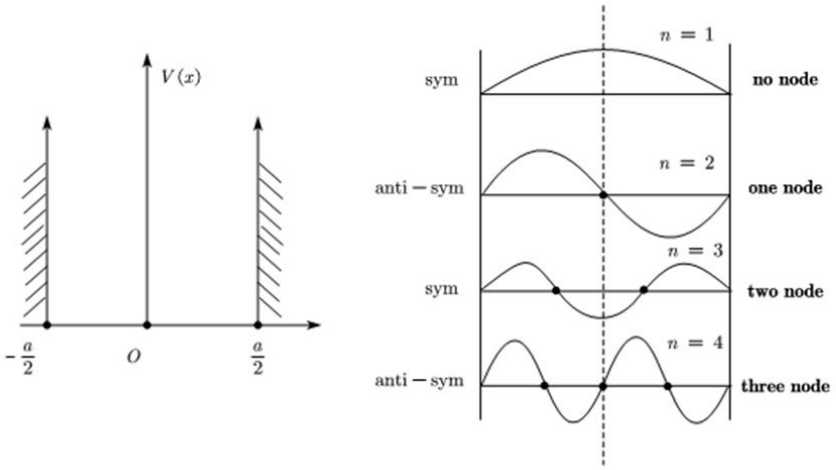


Fig. 4: Infinite Square Well

• Solution: Bound State Solution; discrete; energy $E < 0$. $(E = -|E|)$

even solution:

$$\xi^2 + \eta^2 = Z_0^2,\ \xi = \eta \tan \eta. \quad (\xi, \eta > 0).$$

odd solution:

$$\xi^2 + \eta^2 = Z_0^2,\ \xi = -\eta \cot \eta. \quad (\xi, \eta > 0).$$

$$\begin{cases} \xi = ka = \sqrt{\dfrac{2m}{\hbar^2}(V_0 - |E|)} \cdot a, \\ \eta = \kappa a = \sqrt{\dfrac{2m|E|}{\hbar^2}} \cdot a, \\ Z_0^2 = \dfrac{2mV_0a^2}{\hbar^2}. \end{cases}$$

• Nodes：

$\psi_n(x)$ has $(n-1)$ nodes. [No nodes for ground state]

Exponetial decay: ground state $\leftrightarrow$ fastest.

• Boundary condition:

$$\begin{cases} \psi(x) \text{ continuous at } x = a; \\ \psi'(x) \text{ continuous at } x = a. \end{cases}$$

1) $-V_0 < E < 0 \ \Rightarrow\ \tilde{E} = E - (-V_0) = E + V_0 = V_0 - |E| > 0$

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{2m}{\hbar^2}(E - V(x))\psi = \tilde{k}(x)\psi.$$

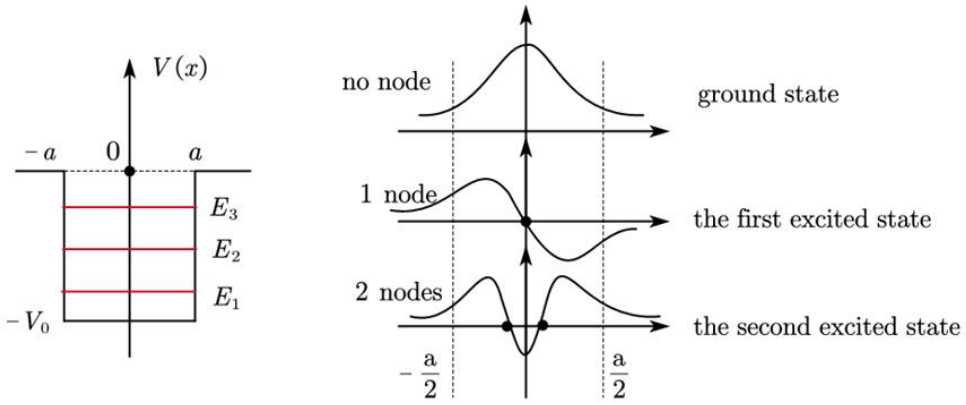


Fig. 5: Finite Square Well

$$\begin{cases} |x| > a: \ \tilde{k}(x) > 0 \text{ (since } E < 0) \ \Rightarrow \text{ expotential wavefunction } \psi(x) \text{ (no parity.)} \\ |x| < a: \ \tilde{k}(x) < 0 \text{ (since } E - V > 0) \ \Rightarrow \text{ trigonometric wavefunction } \psi(x) \text{ (explicit parity.)} \end{cases}$$

$V(-x) = V(x) \ \Rightarrow \ \hat{H}$ has even parity $\Rightarrow$ wavefunction has explicit parity.

2) Even parity solution case:

When $|x| < a$:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = -\frac{2m}{\hbar^2}\Big(E - V(x)\Big)\psi = -\frac{2m}{\hbar^2}(V_0 - |E|)\psi = -k^2\psi.$$

where $k^2 = \dfrac{2m}{\hbar^2}(V_0 - |E|) > 0, \ (k > 0).$

$\Rightarrow \ \psi''(x) = -k^2\psi(x) \ \Rightarrow \ \psi(x) \sim \cos kx. \quad (|x| < a).$

When $|x| > a$:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = -\frac{2m}{\hbar^2}E\psi = \frac{2m|E|}{\hbar^2}\psi = \kappa^2\psi.$$

where $\kappa^2 = \dfrac{2m|E|}{\hbar^2} > 0, \ (\kappa > 0) \Rightarrow \psi''(x) = \kappa^2\psi \ \Rightarrow \psi(x) = Ae^{-\kappa|x|} \ (|x| > a).$

It should be noted that:

$$k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2} \ \Rightarrow \ k^2a^2 + \kappa^2a^2 = \frac{2mV_0a^2}{\hbar^2}.$$

Define dimensionless constants:

$$\eta = ka > 0, \ \xi = \kappa a > 0, \ Z_0^2 = \frac{2mV_0a^2}{\hbar^2} \ \Rightarrow \ \eta^2 + \xi^2 = Z_0^2.$$

$$\xi^2 = \kappa^2 a^2 = \frac{2m|E|a^2}{\hbar^2} = \frac{2mV_0a^2}{\hbar^2}\frac{|E|}{V_0} = Z_0^2\frac{|E|}{V_0} \;\Rightarrow\; \frac{|E|}{V_0} = \Big(\frac{\xi}{Z_0}\Big)^2.$$
$$\eta^2 = k^2a^2 = \frac{2ma^2}{\hbar^2}(V_0 - |E|) = \frac{2ma^2}{\hbar^2}\cdot\tilde{E} \;\Rightarrow\; \tilde{E} = V_0 - |E| = \eta^2\Big(\frac{\hbar^2}{2ma^2}\Big).$$

Continuity of Boundary Condition:

$\psi(x), \psi'(x)$ are continuous at $x = a$,

$$\begin{cases} \psi \text{ continuous at } x = a \;\Rightarrow\; \cos(ka) = Ae^{-\kappa a}; \\ \psi' \text{ continuous at } x = a \;\Rightarrow\; -k\sin(ka) = -\kappa Ae^{-\kappa a}. \end{cases}$$

$$\Longrightarrow \quad \frac{-k\sin(ka)}{\cos(ka)} = \frac{-\kappa Ae^{-\kappa a}}{Ae^{-\kappa a}} \;\Rightarrow\; k\tan(ka) = \kappa.$$
$$\Longrightarrow \quad (ka)\tan(ka) = \kappa a \;\Rightarrow\; \xi = \eta\tan\eta, \quad (\xi, \eta > 0).$$

So, for even solution:

$$\xi^2 + \eta^2 = Z_0^2, \quad \xi = \eta\tan\eta.$$

Deepest bound state = lowest η;

Z_0 : controls the number of even bound states.

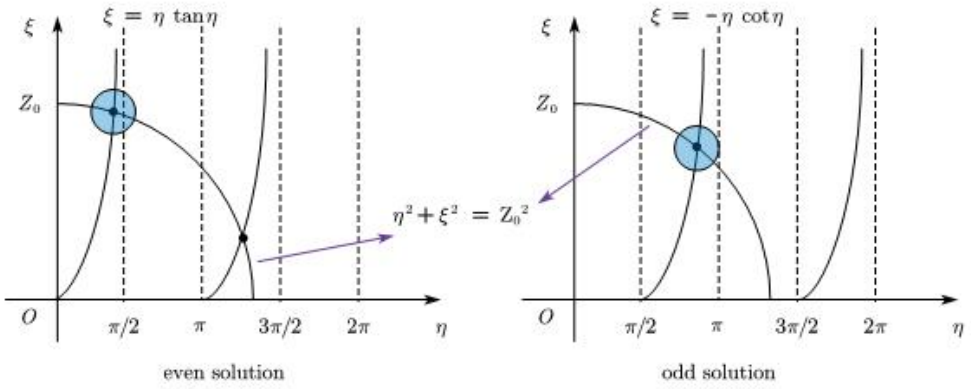


Fig. 6: solutions for 1D finite square well

3) Odd parity solution case:

$$\psi(x) = \begin{cases} \sin(kx), & |x| < a; \\ Ae^{-\kappa|x|}, & |x| > a. \end{cases}$$

Continuity of Boundary Condition:

$\psi(x),\ \psi'(x)$ are continuous at $x = a$,

$$\begin{cases} \psi \text{ continuous at } x = a \ \Rightarrow\ \sin(ka) = Ae^{-\kappa a}; \\ \psi' \text{ continuous at } x = a \ \Rightarrow\ k\cos(ka) = -\kappa A e^{-\kappa a}. \end{cases}$$

$$\Longrightarrow \quad \frac{k\cos(ka)}{\sin(ka)} = \frac{-\kappa A e^{-\kappa a}}{Ae^{-\kappa a}} \ \Rightarrow\ -k\cot(ka) = \kappa.$$

$$\Longrightarrow \quad -(ka)\cot(ka) = \kappa a \ \Rightarrow\ \xi = -\eta\cot\eta, \quad (\xi, \eta > 0).$$

Only one odd bound state $\in [\pi/2, 3\pi/2]$.

No odd bound state $\in [0, \pi/2]$ and $\in [3\pi/2, 2\pi]$.

Exercises:

1. If the potential is:

$$V(x) = \begin{cases} \infty, & (x > a \text{ or } x < 0); \\ 0. & (0 < x < a) \end{cases}$$

Find the solution of the square well. Can you find any parity properties in this case? Is this the same as the 1D infinite well problem of this lecture?

2. 1D infinite square well vs. 1D harmonic oscillator.
3. 1D $\delta-$potential well vs. 1D infinite well.
4. 1D $\delta-$potential barrier vs. 1D infinite barrier.
5. 1D square well vs. Coloumb potential problem.

Lecture Notes 16 Barrier Problem

Contents

- Two Main Problems;
- Step Potential;
- Finite Square Barrier;
- General Discussions of SSE (1D);
- Wavefunction Behavior in Different Regions.

1. Pereliminaries

We have two main problems to solve in QM:

(1) Well Problem（势阱问题）:

$$\text{Bound Problem} \quad \Rightarrow \begin{cases} \text{1D finite well} \\ \text{1D infinite well} \end{cases} \Leftarrow \begin{cases} \text{known: } V(x); \\ \text{unknown: } E, \psi(x). \end{cases}$$

(2) Barrier Problem（势垒问题）:

$$\text{Scattering Problem} \quad \Rightarrow \begin{cases} \text{1D Step Potential} \\ \text{1D Infinite Space Barrier} \end{cases} \Leftarrow \begin{cases} \text{known: } V(x), E; \\ \text{unknown: } \psi(x). \end{cases}$$

2. Step Potential

Solutions to SSE (stationary Schrödinger equation) with step potential are sactteringing states of definite energy E.

$$\text{Two cases} \begin{cases} E > V_0\text{: classically allowed.} \\ E < V_0\text{: classically forbidden.} \end{cases}$$

Step Potential is like:

$$V(x)=\begin{cases}0, & (x<0)\\ V_0, & (x\geqslant 0)\end{cases}$$

It is **NOT** normalizable when $x\to\infty$.

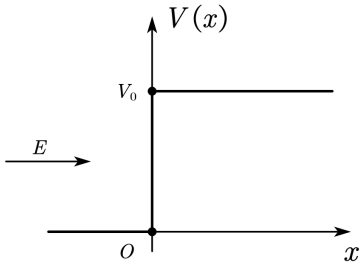


Fig. 7: step function barrier

We know that in SSE,

$$\Psi(x,t)=\psi(x)e^{-iEt/\hbar}.$$

In the following, We try to find $\psi(x)$ in the following discussions.

- $E>V_0$ case:

  SSE:

$$\boxed{\psi''=-\frac{2m(E-V(x))}{\hbar^2}\psi.}$$

Solution:

$$\boxed{\psi(x)=\begin{cases}\underline{Ae^{ikx}} & + & \underline{Be^{-ikx}}, & (x<0)\\ \text{(incident wave)} & & \text{(reflected wave)} & \\ \underline{Ce^{ik'x}}, & & & (x>0)\\ \text{(transmitted wave)} & & & \end{cases}}$$

where

$$k^2=\frac{2mE}{\hbar^2};\quad k'^2=\frac{2m(E-V_0)}{\hbar^2}$$

are two wave vectors.

Considering boundary conditions, $\psi(x)$ and $\psi'(x)$ must be continuous at $x=0$:

$$\begin{cases}\psi(0^+)=\psi(0^-)\Rightarrow & C=A+B,\\ \psi'(0^+)=\psi'(0^-)\Rightarrow & ik'C=ik(A-B).\end{cases}$$

$$\Rightarrow\begin{cases}A-B=\dfrac{k'}{k}C,\\ A+B=C,\end{cases}\Rightarrow\begin{cases}\dfrac{B}{A}=\dfrac{k-k'}{k+k'},\\ \dfrac{C}{A}=\dfrac{2k}{k+k'}.\end{cases}\quad(A,B,C\in\mathbb{R})$$

Analysis of current density: $\boxed{\boldsymbol{j}=\frac{\hbar}{m}\mathrm{Im}(\psi^*\nabla\psi).}$

For $E = V_0 \Rightarrow k' = 0 \Rightarrow B = A, C = 2A$.
So, for $E = V_0$, the energy eigenstates is:

$$\psi(x) = \begin{cases} 2A\cos(kx), & (x < 0) \\ 2A. & (x > 0) \end{cases}$$

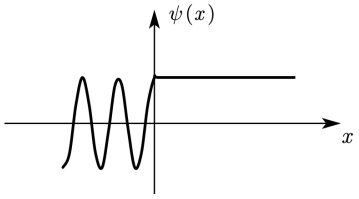


Fig. 8: wave function when $E = V_0$.

According to SE, we have

$$\begin{cases} \dfrac{\partial}{\partial t}\psi(x) = -\dfrac{\hbar}{2mi}\nabla^2\psi - \dfrac{1}{i\hbar}V(x)\psi(x), \\ \dfrac{\partial}{\partial t}\psi^*(x) = +\dfrac{\hbar}{2mi}\nabla^2\psi^* + \dfrac{1}{i\hbar}V(x)\psi^*(x). \end{cases} \Longrightarrow \quad \frac{\partial}{\partial t}(|\psi|^2) = -\frac{\hbar}{2mi}\nabla\cdot(\psi^*\nabla\psi - \psi\nabla\psi^*).$$

According to the current conservation:

$$\frac{\partial\rho}{\partial \mathrm{t}} + \nabla\cdot\boldsymbol{j} = 0, \text{ where } \boxed{\boldsymbol{j} = \frac{h}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*).}$$

Let $\psi^*\nabla\psi = c = a + ib$, so $\psi\nabla\psi^* = c^* = a - ib$, then one has

$$\psi^*\nabla\psi - \psi\nabla\psi^* = 2ib = 2i\cdot\mathrm{Im}(\psi^*\nabla\psi).$$

Hence,

$$\boxed{\boldsymbol{j} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*) = \frac{\hbar}{m}\mathrm{Im}(\psi^*\nabla\psi).}$$

So we have:

$$\begin{aligned} \psi_L(x) &= Ae^{ikx} + Be^{-ikx} \\ \Rightarrow \boldsymbol{J}_L &= \frac{\hbar}{m}\mathrm{Im}\Big(\psi_L^*\frac{\mathrm{d}}{\mathrm{d}x}\psi_L\Big) \\ &= \frac{\hbar}{m}\mathrm{Im}\Big[(Ae^{-ikx} + Be^{ikx})ik(Ae^{ikx} - Be^{-ikx})\Big] \\ &= \frac{\hbar k}{m}\Big[|A|^2 - |B|^2\Big]. \end{aligned}$$

We can also write the current density of "reflected" and "incident" terms.

$$\begin{cases} \psi_A = Ae^{ikx} \Rightarrow J_A = \dfrac{\hbar}{m}\mathrm{Im}\Big(\psi_A^*\dfrac{\mathrm{d}}{\mathrm{d}x}\psi_A\Big) = \dfrac{\hbar k}{m}|A|^2, \\ \psi_B = Be^{-ikx} \Rightarrow J_B = \dfrac{\hbar}{m}\mathrm{Im}\Big(\psi_B^*\dfrac{\mathrm{d}}{\mathrm{d}x}\psi_B\Big) = \dfrac{\hbar k}{m}|B|^2. \end{cases}$$

So we can find that:

$$J_L = J_A - J_B.$$

Also, we can derive the transmitted term like:

$$J_R = \frac{\hbar}{m}\mathrm{Im}(\psi_R^* \frac{\mathrm{d}}{\mathrm{d}x}\psi_R) = \frac{\hbar k'}{m}|C|^2 = J_C.$$

From $\boldsymbol{\nabla} \cdot \boldsymbol{J} = \dfrac{\mathrm{d}}{\mathrm{d}x} J \equiv 0$, we have:

$$\boxed{J_L = J_R.}$$

From the above results, we can derive another constraint:

$$\frac{\hbar k}{m}(|A|^2 - |B|^2) = \frac{\hbar k}{m}\Big[1 - \Big(\frac{k-k'}{k+k'}\Big)^2\Big]|A|^2 = \frac{\hbar k}{m} \cdot \frac{4kk'}{(k+k')^2}|A|^2 = \frac{\hbar k'}{m}|C|^2.$$

So we can have:

$$\frac{4k^2}{(k+k')^2}|A|^2 = |C|^2 \overset{\text{also}}{\Longrightarrow} \frac{C}{A} = \frac{2k}{k+k'}.$$

We derive the following relation before:

$$J_A - J_B = J_C \Rightarrow 1 = \frac{J_B}{J_A} + \frac{J_C}{J_A}.$$

So we can define two important coefficients:

$$\text{Reflection coefficient: } R = \frac{J_B}{J_A} = \frac{|B|^2}{|A|^2} = \Big(\frac{k-k'}{k+k'}\Big)^2 \leqslant 1;$$

$$\text{Transmission coefficient: } T = \frac{J_C}{J_A} = \frac{k'}{k}\frac{|C|^2}{|A|^2} = \frac{k'}{k}\frac{4k^2}{(k+k')^2} = \frac{4kk'}{(k+k')^2} \neq \frac{|C|^2}{|A|^2}.$$

And we have:

$$\boxed{R + T = \frac{4kk'}{(k+k')^2} + \Big(\frac{k-k'}{k+k'}\Big)^2 = 1.}$$

When $E = V_0$, $k' = 0$, we have full relection: $\begin{cases} R = 1, \\ T = 0, \end{cases}$ and

$$J_C = \frac{\hbar k'}{m}|C|^2 \equiv 0.$$

That means no current density on the right when $E = V_0$.

• $E < V_0$ case:

$x > 0$: classical forbidden region. In QM, we have the solution:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & (x < 0), \quad \text{where } k^2 = \dfrac{2mE}{\hbar^2}. \\ Ce^{ik'x}. & (x > 0), \quad \text{where } k'^2 = \dfrac{2m(E - V_0)}{\hbar^2} = (i\kappa)^2. \end{cases}$$

So, for $x > 0$, rewrite $\psi(x)$:

$$\psi(x) = Ce^{-\kappa x}, \qquad \kappa^2 = \frac{2m(V_0 - E)}{\hbar}.$$

$$\Rightarrow \quad \boxed{\frac{B}{A} = \frac{k - i\kappa}{k + i\kappa} = -\frac{\kappa + ik}{\kappa - ik} = -e^{2i\theta(E)},} \quad \text{where } \theta(E) = \tan^{-1}\left(\frac{k}{\kappa}\right) = \tan^{-1}\left(\sqrt{\frac{E}{V_0 - E}}\right).$$

That is, magnitude of A = magnitude of $B = \sqrt{k^2 + \kappa^2}$. So we have:

$$\begin{cases} J_A = J_B = \dfrac{\hbar k}{m}(k^2 + \kappa^2). \\ J_C = \dfrac{\hbar}{m}\mathrm{Im}\Big[C^* e^{-\kappa x}(-\kappa)Ce^{-\kappa x}\Big] = \dfrac{\hbar}{m}\mathrm{Im}(\text{real number}) \equiv 0. \end{cases}$$

Note that for $E < V_0$: $\boxed{T = 0; R = 1}$ $\Rightarrow$ B/A is a pure phase $-e^{2i\theta}$. Phase of the $\begin{cases} \text{numerator } = \kappa + ik = e^{i\theta(E)}, \\ \text{denominator } = \kappa - ik = e^{-i\theta(E)}. \end{cases}$, where $\theta(E) = \tan^{-1}\left(\sqrt{\dfrac{E}{V_0 - E}}\right) = \begin{cases} \xrightarrow{E\to\infty} 0, \\ \xrightarrow{E\to V_0} \pi/2. \end{cases}$

Total wavefuction for $x < 0$:

$$\begin{aligned} \psi(x) &= Ae^{ikx} + Be^{-ikx} = Ae^{ikx} - Ae^{2i\theta(E)}e^{-ikx} \\ &= Ae^{i\theta(E)}[e^{-i\theta(E)}e^{ikx} - e^{i\theta(E)}e^{-ikx}] \\ &= 2iAe^{i\theta(E)} \cdot \sin(kx - \theta(E)). \\ \Rightarrow &\boxed{|\psi(x)|^2 = 4A^2 \sin^2(kx - \theta(E)).} \end{aligned}$$

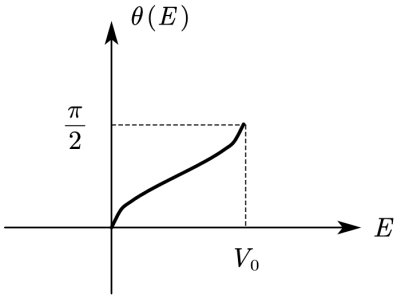


Fig. 9: Energy dependence of the phase.

In the region $x > 0$, we have tunneling effect:

$$\psi(x) = Ce^{-\kappa x}.$$

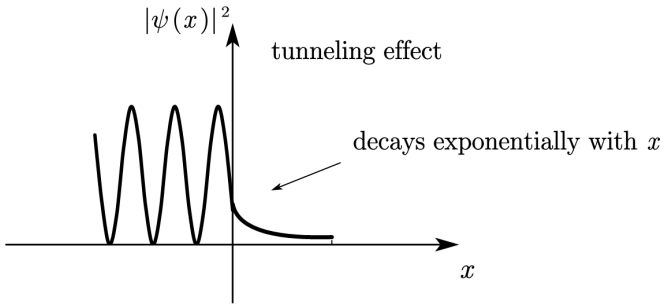


Fig. 10: Tunneling effect in this barrier

the penetration depth is defined as: $d_p \sim 1/\kappa$.

$$\kappa^2 = \frac{2m(V_0 - E)}{\hbar^2} \Rightarrow d_p \sim \frac{\hbar}{\sqrt{2m(V_0 - E)}}.$$

Discussion:

(1) the particle in forbidden region, its position uncertainty must be $\Delta x \leqslant d_{\mathrm{p}}$:

$$\Delta x \sim d_{\mathrm{p}} = \frac{\hbar}{\sqrt{2m(V_0 - E)}} = \frac{1}{\kappa}.$$

(2) the particle acquires some momentum due to position measurement:

$$p \geqslant \frac{\hbar}{\Delta x} \geqslant \frac{\hbar}{d_p} = \hbar\kappa.$$

(3) position measurement $\xrightarrow{induce}$ momentum $p \Longrightarrow$ additional E':

$$E' = \frac{p^2}{2m} \geqslant \frac{\hbar^2\kappa^2}{2m} = \frac{\hbar^2}{2m} \cdot \frac{2m(V_0 - E)}{\hbar^2} = V_0 - E,$$

so we have:

$$E_{\mathrm{tot}} = E + E' \geqslant E + V_0 - E = V_0.$$

This heuristic argument gives some evidence that NO negative kinetic energy will be detected for a particle that is found in the forbiddent region.

3. Finite Square Barrier (Continuous Spectrum; Unbounded State)

(1) Potential:

$$V(x) = \begin{cases} V_0, & (0 \leqslant x \leqslant a), \\ 0, & (x < 0 \text{ or } x > a). \end{cases}$$

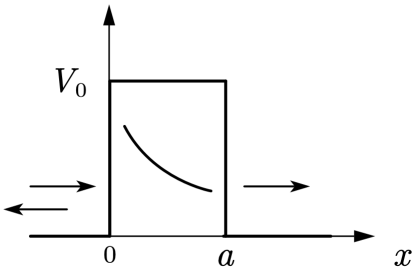


Fig. 11: 1D Finite barrier

(2) SSE: Only consider the case of $E < V_0$:

$$\begin{cases} \psi'' = \dfrac{2m}{\hbar}(V_0 - E)\psi = \kappa^2\psi, & (0 \leqslant x \leqslant a), \\ \psi'' = -\dfrac{2mE}{\hbar^2}\psi = -k^2\psi, & (x < 0 \text{ or } x > a), \end{cases}$$

where

$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}, \quad k = \frac{\sqrt{2mE}}{\hbar}.$$

The solution is:

$$\boxed{\psi(x) = \begin{cases} Ae^{\kappa x} + Be^{-\kappa x}, & (0 < x < a), \\ e^{ikx} + Qe^{-ikx}, & (x < 0), \\ Se^{ikx}. & (x > a). \end{cases}}$$

(3) Boundary Condition:

$\psi(x)$ and $\psi'(x)$ are continuous at $x = 0$, and $x = a$.

$$\Longrightarrow \quad \begin{cases} 1 + Q = A + B, & \left(\psi(0^+) = \psi(0^-)\right) \\ \dfrac{ik}{\kappa}(1 - Q) = A - B, & \left(\psi'(0^+) = \psi'(0^-)\right) \end{cases}$$

$$\Longrightarrow \quad \begin{cases} Ae^{\kappa a} + Be^{-\kappa a} = Se^{ika}, & \left(\psi(a^+) = \psi(a^-)\right) \\ Ae^{\kappa a} - Be^{-\kappa a} = \dfrac{ik}{\kappa}Se^{ika}. & \left(\psi'(a^+) = \psi'(a^-)\right) \end{cases}$$

and then one yields:

$$\begin{cases} T = |S|^2 = \dfrac{4k^2\kappa^2}{(k^2+\kappa^2)^2 2\hbar^2\kappa a + 4k^2\kappa^2}, \\ R = |Q|^2 = \dfrac{(k^2+\kappa^2)^2 2\hbar^2\kappa a}{(k^2+\kappa^2)^2 2\hbar^2\kappa a + 4k^2\kappa^2}, \end{cases}$$

From which yields:

$$R + T = 1.$$

• Discussions:

(1) Though $E < V_0$, there still has the result of $T \neq 0$. This is the **quantum tunneling effect**.

(2) When $E \ll V_0$, yeilds:

$$T \ \to \ \frac{16E(V_0-E)}{V_0^2}\exp\left[-\frac{2a}{\hbar}\sqrt{2m(V_0-E)}\right] \ \to \ 0.$$

This can be used to explain the $\alpha-$decay for radioactive elements (Gamow effect).

(3) When $E > V_0$, yeilds

$$T = \frac{1}{1+\frac{1}{4}(\frac{k}{k'}-\frac{k'}{k})^2\sin^2 k'a} = \frac{1}{1-\frac{1}{4}(\frac{k}{\kappa}+\frac{\kappa}{k})^2\sin^2(-i\kappa a)} \neq 1.$$

$\Rightarrow$ Tunneling effect leads to an uncomplete transmission even though the energy is higher than the potential barrier.

	QM vs. CM	
$E > V_0$	$\begin{cases}\text{partial transmission}\\ \text{partial reflection}\end{cases}$	complete transmission
$E < V_0$	$\begin{cases}\text{partial transmission}\\ \text{partial reflection}\end{cases}$	complete reflection

4. General Discussions of SSE (1D):

• **Theorem/ Corollaries:**

Theorem 1: If $V(x) \in \mathbb{R}$, then $\psi(x)$ can be chosen to be real.

[**Proof**]

Suppose $\psi(x)$ is a solution of SSE, then, so is ψ^*.

$$\psi'' + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0 \;\Rightarrow\; \psi^{*''} + \frac{2m}{\hbar^2}(E - V(x))\psi^* = 0.$$

Hence, $\psi_{\mathrm{R}} = \frac{1}{2}(\psi + \psi^*), \psi_{\mathrm{I}} = \frac{1}{2i}(\psi - \psi^*)$ are also the solutions of SSE.

Solution of SSE: $\psi(x), \psi^*(x), \psi_{\mathrm{R}}(x) \in \mathbb{R}, \psi_{\mathrm{I}}(x) \in \mathbb{R}$.

If $\psi^* = c\psi \Rightarrow \frac{\psi^*}{\psi} = c = e^{-2i\theta} \Rightarrow\; |c|^2 = 1$, just a global phase factor.

Therefore, the solution of SSE can be chosen to be real.

That is to say, for the bound state of 1-D potential (real potential), the solution can be chosen to be **Real**.

Corollary 1: Any bound state $\psi(x)$ of a 1-D potential is real up to a global phase.

[**Proof**]

1D real potential $\Rightarrow$ no degeneracy

$\Rightarrow\; \psi_{\mathrm{I}}(x) = c\psi_{\mathrm{R}}(x) \;\Rightarrow\; \psi(x) = \psi_{\mathrm{R}}(x) + i\psi_{\mathrm{I}}(x) = (1 + ic)\psi_{\mathrm{R}}(x),\; c \in \mathbb{R}$

$= \sqrt{1 + c^2}e^{i\beta} \cdot \psi_{\mathrm{R}}(x) \;\Rightarrow\; \psi(x)$ is real except phase factor $e^{i\beta}$.

Theorem 2: If $V(-x) = V(x)$ (even potential), the eigenstates of Hamiltonian can be chosen to be even or odd under $x \to -x$.

[**Proof**]

$$\psi'' + \frac{2m}{\hbar^2}(E - V(x))\psi = 0 \;\Rightarrow\; \psi''(-x) + \frac{2m}{\hbar^2}(E - V(x))\psi(-x) = 0.$$

Let $\psi_S(x) = \dfrac{\psi(x) + \psi(-x)}{2},\; \psi_A(x) = \dfrac{\psi(x) - \psi(-x)}{2},$

$\Rightarrow\; \psi_S(x), \psi_A(x)$ exist and are the solution of SSE.

Corollary 2: Any bound state of 1-D even potential, No degeneracy $\Rightarrow$ solutions $\psi(x)$ are automatically even or odd.

Absence of degeneracy $\Rightarrow \psi(x), \psi(-x)$ are solution.

From Corollaryly 1, $\psi(x) \in \mathbb{R}$, then $\psi(-x) = c\psi(x),\; (c \in \mathbb{R})$.

$$\Rightarrow\; \psi(x) = c\psi(-x) = c^2\psi(x) \;\Rightarrow\; c^2 = 1 \;\Rightarrow\; c = \pm 1 \begin{cases} c = +1, \text{ (even)} \\ c = -1, \text{ (odd)} \end{cases}$$

Wavefunction Behavior in Different Regions

SSE:

$$\boxed{\frac{\psi''(x)}{\psi(x)} = -\frac{2m}{\hbar^2}(E - V(x)).}$$

- Discussions:

(1) $E - V(x) < 0$: Classically forbidden region.

$$\frac{\psi''(x)}{\psi(x)} = -\frac{2m}{\hbar^2}\Big(E - V(x)\Big) > 0 \;\Rightarrow\; \psi''(x), \psi(x) \text{ same signs.}$$

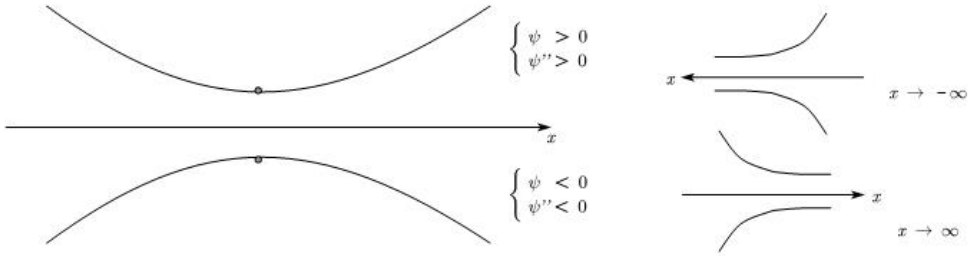


Fig. 12: wave function is convecx (凸) curve towards x axis, and is equal to zero when x approach to infinity.

(2) $E - V(x) > 0$: Classically allowed region

$\psi''(x)$ and $\psi(x)$: opposite signs; wavefunction is concave (凹) towards x axis.

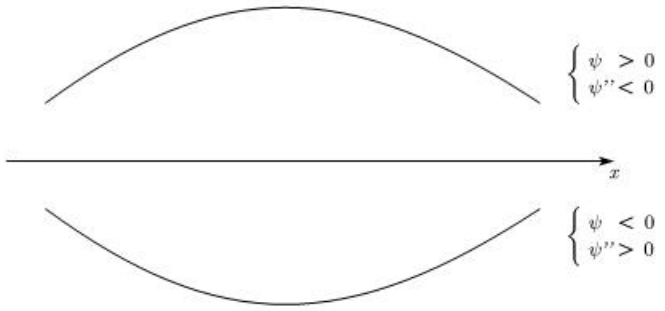


Fig. 13: wave function is concave (凹) curve towards x axis.

(3) $E = V(x_0)$: Tunneling point x_0, is an inflection point (拐点) in curve of $\psi(x)$; $\psi''(x_0) = 0$.

a) Separate classically allowed and classically forbidden region.

b) Not all inflection points are tunneling points.

c) Nodes (节点) are inflection points: $\psi'' = -\frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0 \Rightarrow$ Node: $\psi(x) = 0$。

d) If $\psi' = \psi = 0$, Not allowed ψ.

assume $\exists\ x_0 \Rightarrow \psi'(x_0) = \psi(x_0) = 0 \Rightarrow \psi''(x_0) = 0, \psi^{(3)}(x_0) = 0. \Rightarrow$ Taylor series $= 0 \Rightarrow \psi = 0$.

$$\left(\psi(x) = \psi(x_0) + \psi'(x_0)(x - x_0) + \tfrac{1}{2!}\psi''(x_0)(x - x_0)^2 + \cdots \equiv 0.\right)$$

(4) The Node Theorem (节点定理):

$$\begin{cases} \text{Continuous potential } V(x) \\ V(x) \xrightarrow{|x|\to\infty} \infty \end{cases} \Rightarrow \begin{cases} \text{bound states } \psi_1(x), \psi_2(x), \psi_3(x), \cdots \left(\psi_i(x) \xrightarrow{|x|\to\infty} 0\right) \\ \text{No degeneracy in 1D.} \end{cases}$$

$\Rightarrow$ Node theorem: $\psi_n(x)$ has $(n-1)$ nodes. Example: 1D harmonic oscillator.

Exercises:

1. What will happen when the potential is complex?
2. How to transit from the square potential well to the spherical potential well?

Lecture Notes 17 Quantum Harmonic Oscillator

Contents

- Operators in Quantum Harmonic Oscillator;
- Vacuum state and wavefunction of Fock states.

Introduction

(1D) Harmonic Oscillator is an important and fundamental model in physics. In many problems, we can expand the potential functions using Talor series and approximate them as Harmonic Ocillators, e.g., the particle in potential well, the acoustic phonons, and the particles in electromagnetic fields. The linear harmonic oscillator model is also important in the quantization of the elementary particles (fields).

Basics:

The Hamiltonian of a classical harmonic ocillator (CHO) is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2.$$

Define the length scale $\frac{p^2}{2m} \sim \frac{\hbar^2}{d^2}\frac{1}{2m} \sim \frac{1}{2}m\omega^2 d^2$, we have

$$\frac{\hbar^2}{d^2}\frac{1}{m} \sim m\omega^2 d^2 \Rightarrow d^4 = \frac{\hbar^2}{m^2\omega^2} \Rightarrow d = \sqrt{\frac{\hbar}{m\omega}} \Rightarrow [m\omega^2 d^2] \sim [\hbar\omega].$$

Thus, we have the following relation ($H = E$):

$$1 = \frac{x^2}{(\sqrt{2E/m\omega^2})^2} + \frac{p^2}{(\sqrt{2mE})^2} = \Big(\frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{\hbar}}x + i\frac{1}{\sqrt{2m\hbar\omega}}p\Big)\Big(\frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{\hbar}}x - i\frac{1}{\sqrt{2m\hbar\omega}}p\Big),$$

where we have assumed that $E = \hbar\omega$ in deriving the final equality.

Now we will discuss the operators and states in quantum harmonic oscillator (QHO) problems in detail.

Creation and Annihilation Operator

The relaton derived by the Hamiltonian of a quantum harmonic oscillator is (vs. CHO):

$$\Big(\frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{\hbar}}\hat{x}+i\frac{1}{\sqrt{2m\hbar\omega}}\hat{p}\Big)\Big(\frac{1}{\sqrt{2}}\sqrt{\frac{m\omega}{\hbar}}\hat{x}-i\frac{1}{\sqrt{2m\hbar\omega}}\hat{p}\Big)=1,$$

Define the Creation/Annihilation operator:

- Annihilation Operator（湮灭算符, AO）:

$$\hat{a}=\frac{1}{\sqrt{2}}\left(b_1\hat{x}+ib_2\hat{p}\right).$$

- Creation Operator（产生算符, CO）:

$$\hat{a}^\dagger=\frac{1}{\sqrt{2}}\left(b_1\hat{x}-ib_2\hat{p}\right).$$

where

$$b_1=\sqrt{\frac{m\omega}{\hbar}},\quad b_2=\frac{1}{\sqrt{m\hbar\omega}},\quad [b_1b_2]=[x]^{-1}[p]^{-1}=[L]^{-1}.$$

We can express $\hat{x},\hat{p}$ in linear combination of $\hat{a},\hat{a}^\dagger$:

$$\hat{x}=\frac{1}{\sqrt{2}}\frac{1}{b_1}\left(\hat{a}+\hat{a}^\dagger\right),\quad \hat{p}=\frac{i}{\sqrt{2}}\frac{1}{b_2}\left(\hat{a}^\dagger-\hat{a}\right).$$

From the fundamental commutation relation $[\hat{x},\hat{p}]=i\hbar$, we can get:

$$[\hat{a},\hat{a}^\dagger]=1.$$

So, $\hat{a}\hat{a}^\dagger=\hat{a}^\dagger\hat{a}+1$. Define the Occupation number operator (ONO):

$$\hat{N}=\hat{a}^\dagger\hat{a},$$

we have

$$[\hat{N},\hat{a}]=-\hat{a},\quad [\hat{N},\hat{a}^\dagger]=\hat{a}^\dagger.$$

Let $\hat{N}|\lambda\rangle=\lambda|\lambda\rangle$, we can prove:

$$\hat{N}(\hat{a}|\lambda\rangle)=(\lambda-1)(\hat{a}|\lambda\rangle),\quad \hat{N}\left(\hat{a}^\dagger|\lambda\rangle\right)=(\lambda+1)\left(\hat{a}^\dagger|\lambda\rangle\right).$$

It follows that $\hat{a}|\lambda\rangle$ and $\hat{a}^\dagger|\lambda\rangle$ are also the eigenstates of $\hat{N}$, corresponding to the eigenvalues of $(\lambda-1)$ and $(\lambda+1)$, respectively, i.e.,

$$\hat{a}|\lambda\rangle = C_-|\lambda-1\rangle, \quad \hat{a}^\dagger|\lambda\rangle = C_+|\lambda+1\rangle.$$

Also,

$$\langle\lambda|\hat{a}^\dagger = \langle\lambda-1|C_-^*, \quad \langle\lambda|\hat{a} = \langle\lambda+1|C_+^*.$$

That is why we call $\hat{a}^\dagger$ and $\hat{a}$ as ladder operators. Also, we have

$$|C_-|^2 = \lambda, \quad |C_+|^2 = \lambda+1.$$

Using the phase convention yields

$$\hat{a}|\lambda\rangle = \sqrt{\lambda}|\lambda-1\rangle, \quad \hat{a}^\dagger|\lambda\rangle = \sqrt{\lambda+1}|\lambda+1\rangle.$$

From the

$$\hat{N} = \hat{a}^\dagger\hat{a} = \frac{1}{2}\left(\frac{m\omega}{\hbar}\hat{x}^2 + \frac{1}{m\hbar\omega}\hat{p}^2 - \mathbb{1}\right) \;\Rightarrow\; \hat{H} = \hbar\omega(\hat{N}+\frac{1}{2}).$$

So we have $[\hat{H},\hat{N}]=0$, i.e., $\hat{H},\hat{N}$ have simultaneous eigenstates $|\lambda\rangle$:

$$\hat{H}|\lambda\rangle = \hbar\omega\left(\lambda+\frac{1}{2}\right)|\lambda\rangle.$$

To see what is the value of λ, we can start from $\langle\lambda|\hat{N}|\lambda\rangle = \lambda$, and have:

$$\lambda = \langle\lambda|\hat{N}|\lambda\rangle = \left\langle\lambda\left|\hat{a}^\dagger\hat{a}\right|\lambda\right\rangle = \|\hat{a}|\lambda\rangle\|^2,$$

so we need

$$\lambda \geq 0.$$

Also, since $\hat{a}|\lambda\rangle = \sqrt{\lambda}|\lambda-1\rangle$ and $\hat{a}|0\rangle = \sqrt{0}|0-1\rangle = 0$, we know that minimum of λ is 0. Then we apply the creation operator to $|\lambda\rangle$ to let the eigenvalue increase by 1. Finally, we have $\lambda = n = 0,1,2,3,\cdots$, and

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$

Hence, in particular, note that

$$\hat{a}|0\rangle = 0.$$

Remarks:

1. $\hat{a}^\dagger \neq \hat{a}$, i.e, $\hat{a}^\dagger$ and $\hat{a}$ are not Hermitian.
2. $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \quad (\alpha \in \mathbb{C})$, where $|\alpha\rangle$ is called the coherent state (相干态). Coherent states are the eigenstates of annihilation operator.
3. $\hat{a}^\dagger$ does not have eigenstates.
4. $\hat{N}^\dagger = (\hat{a}^\dagger\hat{a})^\dagger = \hat{a}^\dagger(\hat{a}^\dagger)^\dagger = \hat{a}^\dagger\hat{a} = \hat{N}$, so $\hat{N}$ is hermitian.
5. From $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$, we have

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n|0\rangle, \quad (n = 0,\ 1,\ 2, \cdots).$$

6. From the Hamiltonian $\hat{H} = \dfrac{\hat{p}^2}{2m} + \dfrac{1}{2}m\omega^2\hat{x}^2$, we have

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) = \hbar\omega\left(\hat{N} + \frac{1}{2}\right).$$

so

$$\hat{H}|n\rangle = \hbar\omega(\hat{N} + \frac{1}{2})|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle.$$

and we have

$$\langle\hat{H}\rangle = \langle n|\hat{H}|n\rangle = \hbar\omega(n + \frac{1}{2}) = \langle E\rangle.$$

If $n = 0$，$\langle E\rangle = \dfrac{\hbar\omega}{2}$，is called zero point energy (零点能). The state $|0\rangle$ is called the vacuum state (真空态), and in the following, we will prove that it is a minimum uncertainty state.

Vacuum State and Wavefunction of Fock states

$$\langle n|\hat{N}|n\rangle = \langle n|\hat{a}^\dagger\hat{a}|n\rangle = n,\ \langle n|\hat{H}|n\rangle = \hbar\omega(n + \frac{1}{2}).$$

$$\langle n|\hat{a}|n\rangle = \langle n|\hat{a}^\dagger|n\rangle = 0,\ \langle n|\hat{a}^2|n\rangle = \langle n|\hat{a}^{\dagger 2}|n\rangle = 0.$$

$$\langle n|m\rangle = \delta_{nm};\ \sum_n |n\rangle\langle n| = \mathbb{1}.$$

$$\begin{cases} \hat{a} = \sqrt{\dfrac{m\omega}{2\hbar}}\hat{x} + i\dfrac{1}{\sqrt{2m\hbar\omega}}\hat{p}, \\ \hat{a}^\dagger = \sqrt{\dfrac{m\omega}{2\hbar}}\hat{x} - i\dfrac{1}{\sqrt{2m\hbar\omega}}\hat{p}. \end{cases} \Rightarrow \begin{cases} \hat{x} = \sqrt{\dfrac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right), \\ \hat{p} = i\sqrt{\dfrac{m\hbar\omega}{2}}\left(\hat{a}^\dagger - \hat{a}\right). \end{cases}$$

$$\Longrightarrow \quad \langle\hat{x}\rangle = \left\langle n \left| \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a}+\hat{a}^\dagger\right) \right| n \right\rangle = 0,\ \langle\hat{p}\rangle = i\sqrt{\frac{m\hbar\omega}{2}} \left\langle n \left| \left(\hat{a}^\dagger - \hat{a}\right) \right| n \right\rangle = 0.$$

$$\Longrightarrow \quad \left\langle \hat{x}^2 \right\rangle = \left(\frac{\hbar}{2m\omega}\right) \left\langle n \left| \left(\hat{a}^2 + \hat{a}^{\dagger 2} + 2\hat{a}^\dagger\hat{a} + 1\right) \right| n \right\rangle = \left(\frac{\hbar}{2m\omega}\right)(2n+1) = \frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right);$$

$$\left\langle p^2 \right\rangle = -\left(\frac{m\hbar\omega}{2}\right) \left\langle n \left| \left(\hat{a}^{\dagger 2} + \hat{a}^2 - 2\hat{a}^\dagger\hat{a} - 1\right) \right| n \right\rangle = \frac{m\hbar\omega}{2}(2n+1) = m\hbar\omega\left(n+\frac{1}{2}\right).$$

$$\begin{cases} \Delta\hat{x}^2 = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2 = \langle\hat{x}^2\rangle\,, \\ \Delta\hat{p}^2 = \langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2 = \langle\hat{p}^2\rangle\,. \end{cases}$$

We have:

$$\begin{aligned} \Delta\hat{x}^2\Delta\hat{p}^2 &= \frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right) m\hbar\omega \left(n+\frac{1}{2}\right) \\ &= \hbar^2\left(n+\frac{1}{2}\right)^2. \end{aligned}$$

When $n=0$,

$$\Delta\hat{x}^2\Delta\hat{p}^2 = \frac{\hbar^2}{4}.$$

we have

$$\Delta\hat{x}\ \Delta\hat{p} = \frac{\hbar}{2}.$$

So the vacuum state $|0\rangle$ is the minimum uncertainty state (最小不确定态).

Next we will derive the wavefunction of the Fock state $|n\rangle$ in x-representation: $\psi_n(x) = \langle x|n\rangle$.

Since $\hat{a}|0\rangle = 0$, then

$$\langle x|\hat{a}|0\rangle = \left\langle x \left| \frac{1}{\sqrt{2}}(b_1\hat{x} + ib_2\hat{p}) \right| 0 \right\rangle = 0.$$

Note that

$$\langle x|\hat{x}|\psi\rangle = x\psi(x), \quad \langle x|\hat{p}|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\psi(x),$$

$$\Longrightarrow \quad \sqrt{\frac{m\omega}{2\hbar}}x\langle x|0\rangle + i\frac{1}{\sqrt{2m\hbar\omega}}\left(-i\hbar\frac{\partial}{\partial x}\right)\langle x|0\rangle = 0.$$

$$\Longrightarrow \quad \left[\sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right]\psi_0(x) = 0,$$

$$\Longrightarrow \quad \left(x + \frac{\hbar}{m\omega}\frac{d}{dx}\right)\psi_0(x) = 0,$$

$$\Longrightarrow \quad x\cdot\psi_0 = -\frac{\hbar}{m\omega}\frac{d\psi_0}{dx} \;\Rightarrow\; \frac{d\psi_0(x)}{\psi_0(x)} = -\frac{m\omega}{\hbar}xdx,$$

$$\Longrightarrow \quad \ln\psi_0(x) = -\frac{m\omega}{2\hbar}x^2.$$

So the wavefunction of the ground state $\psi_0(x) = \langle x|0\rangle$ is

$$\psi_0(x) = Ae^{-m\omega x^2/2\hbar},$$

where A is the normalization factor,

$$|A|^2 = \left[\int_{-\infty}^{+\infty} e^{-m\omega x^2/\hbar}dx\right]^{-1} = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}},$$

where we have used the relation

$$\int_{-\infty}^{+\infty} e^{-\alpha x^2}dx = \sqrt{\frac{\pi}{\alpha}}, \quad \alpha = \frac{m\omega}{\hbar}.$$

Let A is real, we have

$$A = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}},$$

so the wavefunction of the ground state is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m\omega x^2/2\hbar}.$$

We can use the creation operator to derive all other excited state wavefunction:

$$\begin{aligned}
\psi_n(x) = \langle x|n\rangle &= \left\langle x\middle|\frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n\middle|0\right\rangle \\
&= \left\langle x\middle|\frac{1}{\sqrt{n!}}\left[\frac{1}{\sqrt{2}}\left(b_1\hat{x} - ib_2\hat{p}\right)\right]^n\middle|0\right\rangle \\
&= \frac{1}{\sqrt{2^n n!}}\left(\frac{mw}{\pi\hbar}\right)^{\frac{1}{4}}\left(\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{\mathrm{d}}{\mathrm{d}x}\right)^n e^{-m\omega x^2/2\hbar} \\
&= \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-m\omega x^2/2\hbar}.
\end{aligned}$$

$H_n(z)$ is Hermite polynomial (厄米多项式). Therefore, it is evident that the wave function of the eigenstates of linear harmonic oscillator are Hermite-Gauss functions.

Exercises:

1. Prove that all the excited state $|n\rangle$ $(n \neq 0)$ is not the minimum uncertainty

state.

2. Show that the creation operator $\hat{a}^\dagger$ does not have eigenstates.

3. Try to represent the coherent state $|\alpha\rangle$ in the combination of Fock states $|n\rangle$.

4. Derive the wave function of the vacuum state of QHO.

5. Derive the wave function of the excited state of QHO.

6. From the Hamiltonian of CHO, what can you derive from the trajectory (轨迹) in phase space?

7. Prove all the commutations in QHO.

8. What is the physical significance of parameter d in the analysis in this lecture?

9. Compare: vacuum state (ground state of QHO) vs. coherent state.

Lecture Notes 18 Central Potential

Contents

- Review of some basics;
- Central potential.

1. Preliminaries

Central potential: radial coordinate-dependent only.

$$V(\boldsymbol{x}) = V(r), \quad r = \sqrt{x^2 + y^2 + z^2}.$$

Spherical coordinates:

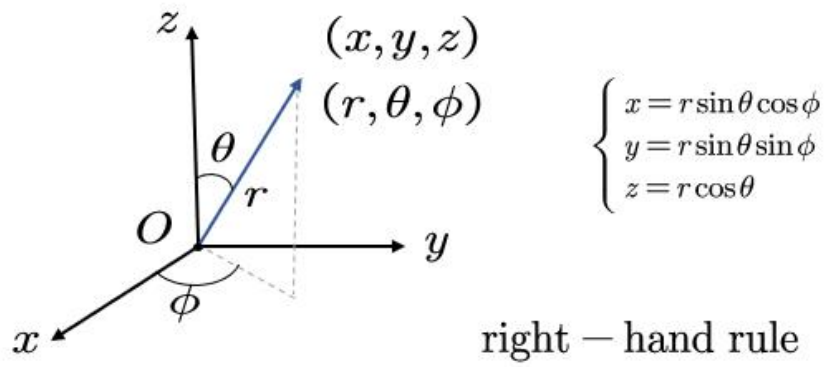


Fig. 14: coordinate system

$$\begin{cases} x = r\sin\theta\cos\phi, \\ y = r\sin\theta\sin\phi, \\ z = r\cos\theta. \end{cases} \Rightarrow \begin{cases} r = \sqrt{x^2 + y^2 + z^2}, \\ \theta = \cos^{-1}\left(\dfrac{z}{\sqrt{x^2 + y^2 + z^2}}\right), \\ \phi = \tan^{-1}\left(\dfrac{y}{x}\right). \end{cases}$$

Classical Mechanics

- Conservation of angular momentum:

$$\frac{d\boldsymbol{L}}{dt} \equiv 0.$$

- Newtonian mechanics:

$$\frac{d\boldsymbol{L}}{dt}=\frac{d}{dt}(\boldsymbol{x}\times\boldsymbol{p})=\frac{d\boldsymbol{x}}{dt}\times\boldsymbol{p}+\boldsymbol{x}\times\frac{d\boldsymbol{p}}{dt},$$

where

$$\frac{d\boldsymbol{x}}{dt}=\boldsymbol{v}\times\boldsymbol{p}=\boldsymbol{v}\times m\boldsymbol{v}\equiv 0,$$

$$\boldsymbol{x}\times\frac{d\boldsymbol{p}}{dt}=\boldsymbol{x}\times(-\boldsymbol{\nabla}V),$$

$$\boldsymbol{\nabla}V=\frac{\partial}{\partial\boldsymbol{x}}V=\frac{dV}{dr}\cdot\frac{\partial r}{\partial\boldsymbol{x}}=\frac{dV}{dr}\cdot\frac{\boldsymbol{x}}{r},$$

$$\boldsymbol{x}\times\frac{d\boldsymbol{p}}{dt}=\boldsymbol{x}\times\left(-\frac{1}{r}\frac{dV}{dr}\boldsymbol{x}\right)=-\frac{1}{r}\frac{dv}{dr}(\boldsymbol{x}\times\boldsymbol{x})=0.$$

- Hamiltonian mechanics:

$$H=\frac{\boldsymbol{p}^2}{2m}+V(r),$$

$$[L_i,H]_{PB}=\left[L_i,\frac{\boldsymbol{p}^2}{2m}\right]_{PB}+\left[L_i,V(r)\right]_{PB},$$

where

$$\begin{aligned}\left[L_i,\frac{\boldsymbol{p}^2}{2m}\right]_{PB}&=\frac{1}{2m}\left[L_i,\boldsymbol{p}^2\right]_{PB}\\&=\frac{1}{2m}\epsilon_{ijk}\left[x_j,\boldsymbol{p}^2\right]_{PB}p_k.\\&=\frac{1}{2m}\epsilon_{ijk}\left(\left[x_j,p_a\right]_{PB}p_a+p_a\left[x_j,p_a\right]_{PB}\right)p_k\\&=\frac{1}{m}\epsilon_{ijk}p_jp_k=0.\end{aligned}$$

$$\begin{aligned}(L_i,V(r)]_{PB}=&[L_i,x_a]_{PB}\frac{\partial V}{\partial x_a}\\=&\epsilon_{ijk}x_j\left[p_k,x_a\right]_{PB}\frac{1}{r}\frac{dV}{dr}\frac{\partial r}{\partial x_a}\\=&\epsilon_{ijk}x_j\left(-\delta_{ak}\right)\frac{1}{r}\frac{dV}{dr}x_a\\=&-\left(\frac{1}{r}\frac{dV}{dr}\right)\epsilon_{ijk}x_jx_k=0.\end{aligned}$$

Quantum Mechanics

$$\hat{H}=\frac{\hat{p}^2}{2m}+V(r),$$

$$\hat{L}_i=\epsilon_{ijk}\hat{x}_j\hat{p}_k;\quad[\hat{x}_i,\hat{p}_j]=i\hbar\delta_{ij}.$$

$$[\hat{A}, f(\hat{B})] = [\hat{A}, \hat{B}]\frac{\partial f}{\partial \hat{B}}.$$

$$\left[\hat{p}_i, \hat{V}(r)\right] = [\hat{p}_i, \hat{x}_a]\,\frac{\partial \hat{V}}{\partial x_a} = -i\hbar\delta_{ia}\cdot\frac{1}{r}\frac{dV}{dr}\hat{x}_a = -\frac{i\hbar}{r}\frac{dV}{dr}\hat{x}_i.$$

$$\left[\hat{L}_i, \frac{\hat{\boldsymbol{p}}^2}{2m}\right] \equiv 0,\ \left[\hat{L}_i, \hat{V}(r)\right] \equiv 0,\ \left[\hat{\boldsymbol{L}}, \hat{V}(r)\right] \equiv 0,\ \left[\hat{\boldsymbol{L}}^2, \hat{H}\right] \equiv 0.$$

2. Central Potential

$$\begin{cases} \left[\hat{L}_i, \hat{H}\right] \equiv 0, \\ \left[\hat{\boldsymbol{L}}^2, \hat{H}\right] \equiv 0. \end{cases}$$

$\hat{\boldsymbol{L}}^2$, $\hat{L}_z$ are both conserved quantities. They have the simultaneous eigenstates of $\hat{H}$. $\left(\hat{H}, \hat{\boldsymbol{L}}^2, \hat{L}_z\right)$ is called the CSCO (complete set of commuting observables). Correspongdingly, there are good quantum numbers l and m_l:

$$\hat{\boldsymbol{L}}^2 \longleftrightarrow l; \quad \hat{L}_z \longleftrightarrow m_l.$$

$$\begin{cases} x = r\sin\theta\cos\phi, \\ y = r\sin\theta\sin\phi, \\ z = r\cos\theta. \end{cases} \Rightarrow \begin{cases} r = \sqrt{x^2+y^2+z^2}, \\ \theta = \cos^{-1}\left(\dfrac{z}{\sqrt{x^2+y^2+z^2}}\right), \\ \phi = \tan^{-1}\left(\dfrac{y}{x}\right). \end{cases}$$

where $x, y, z \in (-\infty, +\infty)$, $r \in [0, \infty)$, $\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$.

Further, one has

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi},$$

$$\hat{\boldsymbol{L}}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right].$$

From the above results, one finds that $\hat{L}_z$ and $\hat{\boldsymbol{L}}^2$ are (θ, ϕ) dependent only (i.e., not dependent on the radial coordinates r).

Angular Momentum

$$\hat{\boldsymbol{L}} = \hat{\boldsymbol{x}} \times \hat{\boldsymbol{p}},$$

$$\hat{L}_i = \epsilon_{ijk}\hat{x}_j\hat{p}_k.$$

$$\begin{cases} \hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = -i\hbar\left(\hat{y}\partial_z - \hat{z}\partial_y\right), \\ \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z = -i\hbar\left(\hat{z}\partial_x - \hat{x}\partial_z\right), \\ \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar\left(\hat{x}\partial_y - \hat{y}\partial_x\right). \end{cases}$$

- The eigenvalue equation of $\hat{\boldsymbol{L}}^2,\ \hat{L}_z$:

$$\begin{cases} \hat{\boldsymbol{L}}^2 \left|l, m_l\right\rangle = \hbar^2 l(l+1) \left|l, m_l\right\rangle, \\ \hat{L}_z \left|l, m_l\right\rangle = \hbar m_l \left|l, m_l\right\rangle. \end{cases}$$

$$\left|l, m_l\right\rangle \xrightarrow{\boldsymbol{x}-\text{representation}} \langle \boldsymbol{x} \mid l m_l\rangle = \langle \theta, \phi \mid l, m_l\rangle = Y_{lm_l}(\theta, \phi). \quad \text{(spherical harmonics)}$$

$$\Longrightarrow \quad \begin{cases} \hat{\boldsymbol{L}}^2 Y_{lm_l}(\theta,\phi) = \hbar^2 l(l+1) Y_{lm_l}(\theta,\phi), \\ \hat{\boldsymbol{L}}_z Y_{lm_l}(\theta,\phi) = \hbar m_l Y_{lm_l}(\theta,\phi). \end{cases}$$

$$\Longrightarrow \quad \begin{cases} -\hbar^2 \left[\dfrac{1}{\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial}{\partial\theta}\right) + \dfrac{1}{\sin^2\theta}\dfrac{\partial^2}{\partial\phi^2}\right] Y_{lm_l}(\theta,\phi) = \hbar^2 l(l+1) Y_{lm_l}(\theta,\phi), \\ -i\hbar\dfrac{\partial}{\partial\phi} Y_{lm_l}(\theta,\phi) = \hbar m_l Y_{lm_l}(\theta,\phi). \end{cases}$$

$$Y_{lm_l} \propto P_l^{m_l}(\cos\theta)\cdot e^{im_l\phi},$$

$$\begin{aligned} Y_{lm_l}(\theta,\phi) &= (-1)^{m_l}\sqrt{\frac{(2l+1)!(l-m_l)!}{4\pi(l+m_l)!}} e^{im_l\phi} P_l^{m_l}(\cos\theta) \\ &= \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(l+m_l)!}{4\pi(l-m_l)!}} e^{im_l\phi}(\sin\theta)^{-m_l}\frac{d^{l-m_l}}{d(\cos\theta)^{l-m_l}}(\sin\theta)^{2l}. \end{aligned}$$

Some useful formulae:

$$\begin{cases} Y_{00}(\theta,\phi) = \dfrac{1}{\sqrt{4\pi}}; \longleftrightarrow |00\rangle = \mid l=0, m=0\rangle, \\ Y_{1\pm1}(\theta,\phi) = \mp\sqrt{\dfrac{3}{8\pi}}\sin\theta\cdot e^{\pm i\phi} = \mp\sqrt{\dfrac{3}{8\pi}}\left(\dfrac{x\pm iy}{r}\right); \longleftrightarrow |1\pm1\rangle = \mid l=1, m=\pm1\rangle, \\ Y_{10}(\theta,\phi) = \sqrt{\dfrac{3}{4\pi}}\cos\theta = \sqrt{\dfrac{3}{4\pi}}\left(\dfrac{z}{r}\right). \longleftrightarrow |10\rangle = |l=1, m=0\rangle. \end{cases}$$

- Orthonormality and resolution of identity:

$$\begin{cases} \langle lm_l | l'm'_{l'}\rangle = \delta_{ll'}\delta_{m_l m'_{l'}}, \\ \displaystyle\sum_{m_l} |lm_l\rangle \langle lm_l| = \mathbb{1}. \end{cases}$$

$$\int \langle lm_l|\boldsymbol{x}\rangle \langle \boldsymbol{x}|l'm'_{l'}\rangle \, d\boldsymbol{x}' = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \cdot Y^*_{lm_l}(\theta,\phi) Y_{l'm'_{l'}}(\theta,\phi) = \delta_{ll'}\delta_{m_l m'_{l'}}.$$

- The Energy Eigenstates

$$\hat{H}|nlm_l\rangle = E_{nlm_l}|nlm_l\rangle.$$

In $\boldsymbol{x}$-representation,

$$\langle \boldsymbol{x}|nlm_l\rangle = \psi_{nlm_l}(r,\theta,\phi) = R_{nl}(r)Y_{lm_l}(\theta,\phi),$$

$$\psi_{nlm_l}(r,\theta,\phi) = R_{nl}(r)Y_{lm_l}(\theta,\phi).$$

$$\left\{-\frac{\hbar^2}{2m}\left[\left(\frac{1}{r}\frac{d^2}{dr}r\right)\right] + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right\} R_{nl}(r) = E_{nl}R_{nl}(r)$$

Let

$$R_{nl}(r) = \frac{1}{r}u_{nl}(r),$$

then

$$\left[-\frac{h^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)h^2}{2mr^2} + V(r)\right] u_{nl}(r) = E_{nl}(r)u_{nl}(r).$$

Since

$$\hat{\boldsymbol{L}}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right],$$

then

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(r) = \frac{\hat{p}_r^2}{2m} + \frac{\hat{\boldsymbol{L}}^2}{2mr} + V(r).$$

Define the ***effective potential***:

$$V_{\text{eff}}(r) = V(r) + \frac{l(l+1)}{2mr^2}\hbar^2,$$

then

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{\text{eff}}(r)\right] u_{nl}(r) = E_{nl}u_{nl}(r).$$

$$V(r) \sim -\frac{1}{r},$$

Since

$$V_{\text{eff}} = V(r) + \frac{l(l+1)h^2}{2m}\frac{1}{r^2} = -A\cdot\frac{1}{r} + B\frac{1}{r^2}.$$

Discussions:

1. when $l = 0$, $V_{\text{eff}}(r) = -\dfrac{A}{r} + 0 = -\dfrac{A}{r}$.
2. when $l > 0$, $V_{\text{eff}}(r) = -\dfrac{A}{r} + B\dfrac{1}{r^2}$.

Asuumption: $|u(r)| < N$ (bounded), $r \to 0$， $r^2 V(r) \xrightarrow{r\to 0} 0$, then we have:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2}\right) u_{nl}(r) = 0, \quad (r \to 0).$$

Then

$$\frac{d^2}{dr^2}u_{nl}(r) = \frac{l(l+1)}{r^2}u_{nl}(r).$$

So,

$$u_{nl}(r) \sim r^\alpha \Rightarrow \frac{d^2}{dr^2}u_{nl} \sim \alpha(\alpha-1)\cdot r^{\alpha-2}, \quad \frac{l(l+1)}{r^2}u_{nl} \sim l(l+1)r^{\alpha-2},$$

$$\alpha(\alpha-1) = l(l+1).$$

$$\Longrightarrow \quad \begin{cases} \alpha = l+1 \Rightarrow u_{nl}(r) = r^{l+1}, \\ \alpha = -l \Rightarrow u_{nl}(r) = r^{-l}. \end{cases}$$

$$\Longrightarrow \quad R_{nl}(r) = \begin{cases} r^l, \\ r^{-l-1}. \end{cases}$$

If $R_{nl}(r) = r^{-l-1}$， then

$$\left.\begin{aligned} \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi), \\ \psi(r,\theta,\phi) = r^{-l-1}\cdot Y_{lm_l}(\theta,\phi), \end{aligned}\right\} \Rightarrow \nabla^2\psi \sim \delta^{(l)}(\boldsymbol{x}).$$

Since

$$\nabla^2\left(\frac{1}{r}\right) = -4\pi\delta(\boldsymbol{x}),$$

then

$$\nabla^2\left[r^{-(l+1)}\right] \sim \delta^{(l)}(\boldsymbol{x}),$$

which is not physically acceptable. So, we adopt that

$$R_{nl} = r^l.$$

when $r \to 0$， $R_{nl}(r) \sim r^l \xrightarrow{r\to 0} 0$， $u_{nl} = r\cdot R_{nl}(r) = r^{l+1} \xrightarrow{r\to\infty} 0$.

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm_l}(\theta,\phi) = N_r r^l \cdot Y_{lm_l}(\theta,\phi).$$

Normalization:

$$\int d^3\boldsymbol{x} \mid \psi_{nlm_l}(r,\theta,\phi)|^2 = 1,$$

$$\Longrightarrow \quad \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \sin\theta \mathrm{d}\theta \cdot |Y_{lm_l}(\theta,\phi)|^2 \cdot \int_0^{\infty} r^2 \mathrm{d}r \cdot |R_{nl}(r)|^2 = 1.$$

For $R_{nl}(r) \sim r^l$, n is the prime quantum number, l is the orbital (azimuthal) angular quantum number. For $Y_{lm_l}(\theta,\phi)$, l is the orbital (azimuthal) angular quantum number, m is the orbital (azimuthal) magnetic quantum number. (For χ_{sm_s}, s represents spin, m_s is the spin magnetic quantum number.)

Exercises:

1. What is the relation between $Y_{lm}(\theta,\phi)$, $Y_{lm}(-\theta,\phi)$ and $Y_{lm}(\theta,-\phi)$?
2. Try to derive Y_{ll} based on the eigenvalue equation.

Lecture Notes 19 Hydrogen Atom (Preliminaries)

Contents

- Center of Mass System;
- Hydrogen Atom and the Radial Parts of Wavefunction;
- Variational Method and Helium Atoms.

1. Basics

- Coloumb's potential: in Gaussian units, the Coloumb's potential is:

$$V(r) = -\frac{e^2}{r}.$$

- Two body systems (TBS): electron and proton (nuclei).

$$e^- : \hat{x}_1, \hat{p}_1, m_1,$$
$$p : \hat{x}_2, \hat{p}_2, m_2.$$

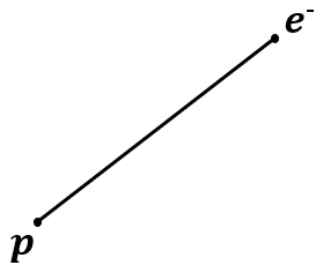


Fig. 15: Two-body system (electron and proton)

$$\hat{H} = \frac{\boldsymbol{p}_1^2}{2m_1} + \frac{\boldsymbol{p}_2^2}{2m_2} + V\left(|\boldsymbol{x}_1 - \boldsymbol{x}_2|\right). \quad (|\boldsymbol{x}_1 - \boldsymbol{x}_2| = r.)$$

- Center of mass system:

$$m_2 \approx 1800 m_1,$$

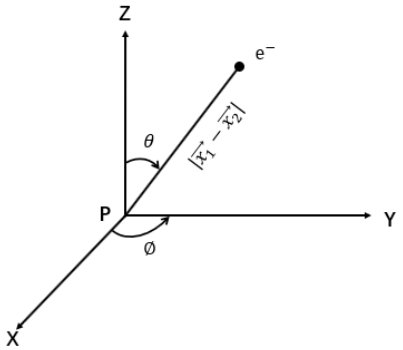


Fig. 16: Hydrogen Atom

reduced mass of the TBS is

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{m_1}{1 + \frac{m_1}{m_2}} = \frac{m_1}{1 + \frac{1}{1800}} \approx m_1.$$

2. Preliminaries

Central potential：

$$\hat{V}(\boldsymbol{x}) = \hat{V}(r),$$

$$[\hat{\boldsymbol{L}}, \hat{H}] \equiv 0,$$

$$\psi(r, \theta, \phi) = R_{nl}(r) Y_{lm_l}(\theta, \phi).$$

Angular momentum：

$$\hat{T} = \frac{\boldsymbol{p}^2}{2m} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{\boldsymbol{L}}^2}{2mr^2},$$

$$\begin{cases} \hat{\boldsymbol{L}}^2 \left| l, m_l \right\rangle = l(l+1)\hbar^2 \left| l, m_l \right\rangle, \\ \hat{L}_z \left| l, m_l \right\rangle = m_l \hbar \left| l, m_l \right\rangle. \end{cases}$$

Center of mass system:

$$e^- : \ \hat{x}_1, \hat{p}_1, m_1, \quad p : \ \hat{x}_2, \hat{p}_2, m_2.$$

$$\hat{H} = \frac{\boldsymbol{p}_1^2}{2m_1} + \frac{\boldsymbol{p}_2^2}{2m_2} + V\left(|\boldsymbol{x}_1 - \boldsymbol{x}_2|\right). \quad (|\boldsymbol{x}_1 - \boldsymbol{x}_2| = r.)$$

Relative coordinates:

$$\boldsymbol{x} = \frac{m_1 \boldsymbol{x}_1 + m_2 \boldsymbol{x}_2}{m_1 + m_2}, \quad \boldsymbol{p} = \boldsymbol{p}_1 + \boldsymbol{p}_2.$$

$$\Longrightarrow \quad \boldsymbol{x} = \boldsymbol{x}_1 - \boldsymbol{x}_2, \quad \boldsymbol{p} = \alpha \boldsymbol{p}_1 - \beta \boldsymbol{p}_2.$$

$$\begin{cases} \boldsymbol{p}_1(\boldsymbol{P}, \boldsymbol{p}), \\ \boldsymbol{p}_2(\boldsymbol{P}, \boldsymbol{p}), \end{cases} \quad \begin{cases} \boldsymbol{x}_1(\boldsymbol{X}, \boldsymbol{x}), \\ \boldsymbol{x}_2(\boldsymbol{X}, \boldsymbol{x}), \end{cases}$$

where $\boldsymbol{P},\ \boldsymbol{X}$ are the momentum and position of the center of mass.

$$[\hat{x}_{ai}, \hat{x}_{bj}] = [\hat{p}_{ai}, \hat{p}_{bj}] \equiv 0.$$

$$[\hat{x}_{ai},\ \hat{p}_{bj}] = i\hbar \delta_{ab} \delta_{ij}.$$

Coefficients:

$$\alpha = \frac{\mu}{m_1},\ \beta = \frac{\mu}{m_2}.$$

Reduced mass:

$$\mu = \frac{m_1 m_2}{m_1 + m_2}.$$

Total mass:

$$M = m_1 + m_2.$$

$$\hat{H} = \frac{\boldsymbol{p}^2}{2\mu} + \frac{\boldsymbol{P}^2}{2M} + V(r).$$

When $m_1 \ll m_2$, $\mu \approx m_1$, the two-body problem is reduced to a one-body probelm.

$$\begin{cases} \dfrac{\boldsymbol{P}^2}{2m} \Psi_{\mathrm{CM}} = E_{\mathrm{CM}} \psi_{\mathrm{CM}}. \\ \left[\dfrac{\boldsymbol{p}^2}{2\mu} + V(|\ \boldsymbol{x}\ |) \right] \Psi_{rel} = E_{rel} \Psi_{rel}. \end{cases}$$

3. Hydrogen atom

Bohr model (semi-classical theory):

$$V(r) = -\frac{e^2}{r}.$$

For hydrogen-like atoms: $-\dfrac{Ze^2}{r}$, Bohr radius: $a_0 = \dfrac{\hbar^2}{me^2} \sim 0.05$ nm.

$$T \sim \frac{1}{2} V,$$

$$E_1 = -\frac{e^2}{2a_0} \sim -13.6\mathrm{eV},$$

$$E_n = E_1 \cdot \frac{1}{n^2} = -\frac{e^2}{2a_0} \cdot \frac{1}{n^2}.$$

So,

$$E_n = -\frac{e^2}{2a_0} \cdot \frac{1}{n^2} = -\frac{e^2}{2 \cdot \left(\frac{\hbar^2}{me^2}\right)} \cdot \frac{1}{n^2} = -\frac{me^4}{2\hbar^2 n^2} \sim \alpha^2 \cdot \left(mc^2\right).$$

Fine Structure Constant (精细结构常数):

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137}, \quad (\text{so, } \alpha^2 = \frac{1}{19000}).$$

For a fixed prime quantum number n, the azimuthal angular quantum number l can take the values of $l = 0, 1, 2 \cdots, n-1$. For a fixed azimuthal angular quantum number l, the azimuthal magnetic quantum number m_l can take the values of $m_l = -l, -l+1, \cdots, l-1, l$. The degeneracy is

$$\sum_{l=0}^{n} (2l+1) = n^2.$$

Considering the spin, the total degeneracy is $2n^2$.

$$\begin{cases} \dfrac{p^2}{2m} \sim \dfrac{\hbar^2}{2m}\nabla^2 \sim \dfrac{\hbar^2}{ma_0^2}. \\ V(r) \sim \dfrac{e^2}{a_0}. \end{cases}$$

The order of magnitude analysis tells that

$$\frac{e^2}{a_0} = \frac{\hbar^2}{ma_0^2} \Rightarrow a_0 = \frac{\hbar^2}{me^2}.$$

• Radial parts of the wavefunction of a hydrogen atom

We discuss the bound state: $E < 0$:

$$u = R(r)/r,$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} - \frac{e^2}{r}\right] u(r) = Eu(r).$$

Let $x = \dfrac{2r}{a_0}$, then

$$\left[-\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2} - \frac{1}{x}\right] u(x) = -\kappa^2 u(x).$$

where

$$\kappa = -\frac{E}{(2e^2/a_0)} = \frac{|E|a_0}{2e^2}.$$

When $x \to \infty$,

$$\frac{d^2u}{dx^2} = \kappa^2 u,$$

so,

$$u \sim e^{\pm\kappa x}.$$

Let $\rho = \kappa x$,

$$\left(-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} - \frac{1}{\kappa\rho}\right) u(\rho) = -u.$$

It follows that

$$\begin{cases} \rho \to \infty, & u \sim e^{-\rho}; \\ \rho \to 0, & u \sim \rho^{l+1}. \end{cases}$$

Hence,

$$u(\rho) = e^{-\rho} \cdot \rho^{l+1} \cdot W(\rho),$$

where

$$W(\rho) = \sum_{k=0}^{\infty} a_k \rho^k.$$

$\exists\ k_{\max},$ s.t., when $k > k_{\max},$ one has $a_k = 0$. Hence,

$$W(\rho) = L_{n_r}^{2n+1}(\rho),$$

where $n = n_r + l + 1$, and $L_{n_r}^{2n+1}$ is Legendre's polynomial.

$$\begin{aligned} &n = 1, 2, 3, \cdots; \\ &n_r = n-1, n-2, \cdots, 0; \\ &l = 0, 1, 2, \cdots, n-1. \end{aligned}$$

• **Summary:**

$$\begin{aligned} E_n &= \kappa^2 \cdot \left(\frac{2e^2}{a_0}\right) \\ &= -\left[\frac{1}{2\left(n_r + l + 1\right)}\right]^2 \left(\frac{2e^2}{a_0}\right) \\ &= -\frac{1}{\left(n_r + l + 1\right)^2} \cdot \left(\frac{2e^2}{a_0}\right) \\ &= -E_1\left(\frac{1}{n^2}\right) \\ &= -13.6 \text{ eV } \left(\frac{1}{n^2}\right). \end{aligned}$$

$$\begin{aligned} \psi_{nlm}(r,\theta,\phi) =& N \cdot \left(\frac{r}{a_0}\right)^l L_{n_r}^{2l+1}(\rho) \cdot e^{-r/na_0} \cdot Y_{lm_l}(\theta,\phi) \\ =& \sqrt{\frac{2}{(na_0)^3}\frac{(n-l-1)!}{2n(l+1)!}} \cdot e^{-\rho} \cdot \rho^l \cdot L_{n_r}^{2l+1}(\rho) \cdot Y_{lm_l}(\theta,\phi), \end{aligned}$$

where $e^{-\rho} = e^{-r/na_0}$; $\rho^l = \left(\frac{r}{na_0}\right)^l$.

4. Calculus of Variations

• **Approximation theory**

1. Perturbation Theory (Non-degenerate and Degenerate);
2. Variational Method;
3. Semi-classical Theory;
4. Other Methods: Scattering, Time-Independent $\cdots$

• **Rayleigh-Ritz Variational Method**

The Expectation of Energy:

$$\begin{cases} \langle \hat{H} \rangle = \langle \psi | \hat{H} | \psi \rangle / \langle \psi | \psi \rangle, \\ \delta \langle \hat{H} \rangle - \lambda \delta(\langle \psi | \psi \rangle) = 0. \end{cases}$$

Ritz Variational Method:

$$\langle \hat{H} \rangle = \frac{\left\langle \psi(c_i) | \hat{H} | \psi\left(c_i\right) \right\rangle}{\langle \psi(c_i) | \psi(c_i) \rangle},$$

$$\delta\langle\hat{H}\rangle = 0 \Rightarrow \sum_i \frac{\partial\langle\hat{H}\rangle}{\partial c_i}\delta c_i \equiv 0.$$

$$\frac{\partial}{\partial c_i}\langle\hat{H}\rangle(c_i) = 0, \qquad c_i \Rightarrow \begin{cases} \langle\hat{H}\rangle, \\ \left|\psi_{(c_i)}\right\rangle\rangle \end{cases}.$$

• Helium Atoms

Hamiltonian:

$$\begin{aligned}\hat{H} &= \left(-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{2e^2}{r_1}\right) + \left(-\frac{\hbar^2}{2m_2}\nabla_2^2 - \frac{2e^2}{r_2}\right) + \frac{e^2}{r_{12}} \\ &= \hat{H}_{0_1} + \hat{H}_{0_2} + \hat{H}_I.\end{aligned}$$

Testing wavefunction:

$$\begin{aligned}\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2) &= \Psi_{100}(\boldsymbol{x}_1)\Psi_{100}(\boldsymbol{x}_2) \\ &= \left\{\frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-\frac{Zr_1}{a_0}}\right\}\left\{\frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-\frac{Zr}{a_0}}\right\} \\ &= \frac{Z^3}{\pi a_0^3} e^{-\frac{Z}{a_0}(r_1+r_2)}.\end{aligned}$$

Hence,

$$\begin{aligned}\langle\hat{H}\rangle(Z) &= \int d^3\hat{x}_1 \int d^3\hat{x}_2 \Psi^*(\boldsymbol{x}_1, \boldsymbol{x}_2)\hat{H}\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2) \\ &= \frac{e^2Z^2}{a_0} - \frac{4e^2Z}{a_0} + \frac{5e^2Z}{8e_0}.\end{aligned}$$

Variation theory gives

$$\frac{\partial}{\partial Z}\langle\hat{H}\rangle = 0 \Rightarrow Z = \frac{27}{16} \approx 1.69,$$

$$E_{\text{ground}} = \frac{e^2}{a_0}\left(Z^2 - 4Z + \frac{5}{8}Z\right) \cong -2.85\left(\frac{e^2}{a_0}\right) = -77\text{eV}.$$

Comparison: using perturbation theory gives:

$$\begin{cases} E_{\text{ground}} \cong -2.75\left(\dfrac{e^2}{a_0}\right) \sim -75\text{eV}. \\ \Psi_{\text{ground}} = \left(\dfrac{27}{16}\right)^3 \dfrac{1}{\pi a_0^3} e^{-\frac{27}{16a_0}(r_1+r_2)}. \end{cases}$$

Exercises:

1. What is the difference between the concepts "difference" (差分) ,"differential" (微分) and "variation" (变分)?

2. Why does there exist a $k_{\max}$ such that when $k > k_{\max}$, all the expansion coefficients $a_k = 0$?

3. What are the properties of Legendre's polynomial?

4. Derive the expressions of some important parameters using Bohr's theory of atom: (1) Bohr radius; (2) 1^{st} ionization energy (第一电离能); (3) Bohr magneton; (4) fine structure constant.

5. In center of mass system, derive all the important results of commutations related to the center of mass and relative coordinates.

6. Try to derive the integral involved in the calculation of Helium atom.

7. Prove that stationary Schrödinger's equation is equivalent to Rayleigh-Ritz variational method.

Lecture Notes 20 Scattering

Contents

- Background of Scattering;
- Schrödinger Equation of the Scattering Problem;
- Hard Sphere Scattering;
- Optical Theorem.

Background of Scattering:

In scattering problem, we do not care too much about the precise solution, but the asymptotic behavior (渐近行为).

The scattering problem is closely related to the collision process. There are three kinds of collision.

(1) Elastic Collision (弹性碰撞):
mechanical energy conservation, depicted by a Local Potential, so is called "Potential Scattering".

$$A + B \longrightarrow A + B.$$

For Central Potensial Scattering: $V(\boldsymbol{x}) = V(r)$.

(2) Inelastic Collision (非弹性碰撞):
cannot be depicted by a potential, general model scattering theory is needed!

$$A + B \longrightarrow A^* + B,$$

where A^* means that particle A in another states (e.g., excited states).

(3) Reaction (反应):
produces different particles, relativistic quantum theory is needed (high energy physics, fundamental particle physics, etc.)

$$A + B \longrightarrow C + D + E + \cdots.$$

Now we illustrate some notes in the scattering problem:

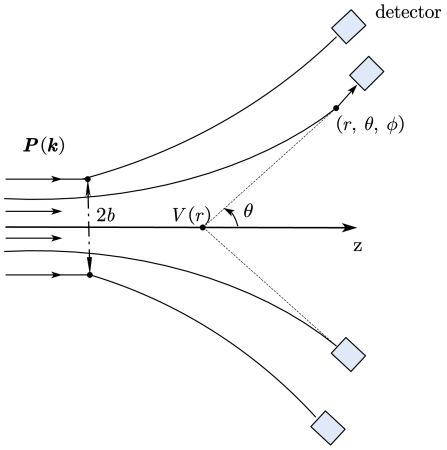


Fig. 17: Shematic of scattering.

θ : deflection (scattering) angle (散射角);
θ, ϕ : azimuthal angle (方位角);
r : radial coordinates (径向坐标);
b : impact parameter (碰撞参数);
$\boldsymbol{k}$: wave number of the incident wave (波数);
$f(\theta, \phi)$: scattering amplitude (散射幅).

• **Important Concepts:**

(1) Probability density (几率密度):

$$\rho = \psi^* \psi.$$

(2) Probability current density (几率流密度):

$$\begin{aligned} \boldsymbol{j} &= -\frac{i\hbar}{2m}(\psi^* \nabla\psi - \psi \nabla\psi^*) \\ &= \frac{\hbar}{m}\mathrm{Im}(\psi^* \nabla\psi) \\ &= \mathrm{Re}\Big[\psi^*\Big(-\frac{i\hbar}{m}\nabla\Big)\psi\Big]. \end{aligned}$$

(3) Current conservation (流守恒) (continuity equation):

The probability flow also satisfies the continuity equation:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot \boldsymbol{j} = 0.$$

When the density of probability remains unchanged (stable), i.e., $\dfrac{\partial \rho}{\partial t} = 0$, then we

have:

$$\nabla \cdot \boldsymbol{j} = -\frac{\partial}{\partial t}\rho = 0.$$

(4) Dimension analysis (量纲分析):

$$\begin{cases} [\rho] = [L]^{-3}, \\ [\boldsymbol{j}] = [L]^{-2}[T]^{-1}. \end{cases}$$

Schrödinger Equation for the Scattering Problem

Form stationary Schrödinger Equation, we have:

$$\Big[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\Big]\psi(\boldsymbol{x}) = E\psi(\boldsymbol{x}), \quad (E > 0).$$

The wavefunction $\psi(\boldsymbol{x})$ is the superpostion of incident and scattering wave, which follows that

$$\psi(\boldsymbol{x}) = \psi_{\text{incident}} + \psi_{\text{scattering}}.$$

Further,

$$\begin{cases} \psi_{\text{incident}} = e^{ikz}, \\ \psi_{\text{scattering}} = \dfrac{e^{ikr}}{r} f(\theta, \phi) + O\Big(\dfrac{1}{r^2}\Big). \end{cases}$$

The above equations mean that the incident wave is a plane wave, while the scattering wave is spherical-like, and $f(\theta, \phi)$ weights the deviation between the scattering wave and the standard spherical wave.

We then analyzes the Hamiltonian in spherical coordinates:

$$\begin{aligned} \nabla^2 &= \frac{1}{r^2}\frac{\partial}{\partial r}\Big(r^2\frac{\partial}{\partial r}\Big) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{r^2\sin\theta}\frac{\partial^2}{\partial\phi^2} \\ &\xrightarrow{r\to\infty} \frac{1}{r^2}\frac{\partial}{\partial r}\Big(r^2\frac{\partial}{\partial r}\Big) + O\Big(\frac{1}{r^2}\Big) = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}. \end{aligned}$$

In far field ($r \to \infty$), one has

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{x}) \sim -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\Big(r^2\frac{\partial}{\partial r}\Big)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi).$$

In stationary case, we start from the continuity equation, and have

$$\nabla \cdot \boldsymbol{j} = 0 \to \oiint \boldsymbol{j} \cdot \mathrm{d}\boldsymbol{\Sigma} = \int_V \nabla \cdot \boldsymbol{j}\mathrm{d}^3\boldsymbol{x} = 0.$$

Consider a tube, through which the probability current flows, then we have:

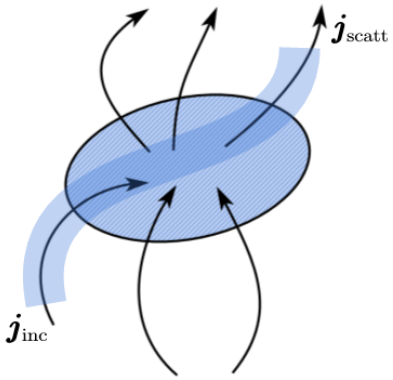


Fig. 18: Conservation of probability flow (continuity).

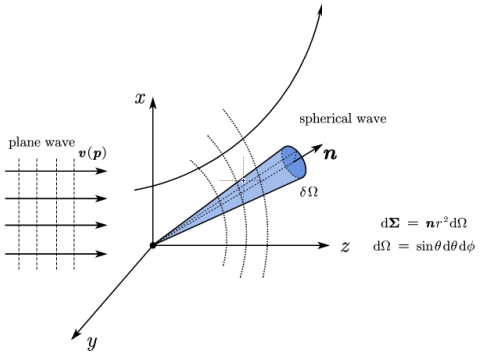


Fig. 19: Schematic of scattering.

$$\boldsymbol{j}_{\text{inc}} \cdot \boldsymbol{\sigma}_{\text{in}} = \boldsymbol{j}_{\text{scatt}} \cdot \boldsymbol{\sigma}_{\text{out}}.$$

The incident wave is a plane wave, which is trivial. Consider the scattering wave:

$$\boldsymbol{j}_{\text{scatt}} = \mathrm{Re}\Big[\psi^*_{\text{scatt}}\Big(\frac{-i\hbar\nabla}{m}\Big)\psi_{\text{scatt}}\Big].$$

In far field, one has

$$\nabla \overset{r\to\infty}{\longrightarrow} \boldsymbol{e}_r\frac{\partial}{\partial r}, \quad \psi_{\text{scatt}} = \frac{e^{ikr}}{r}f(\theta,\phi).$$

It then follows that

$$\boldsymbol{j}_{\text{scatt}} = \boldsymbol{e}_r\Big(\frac{\hbar k}{m}\Big)\frac{|f(\theta,\phi)|^2}{r^2} = \boldsymbol{e}_r\frac{v|\rho(\theta,\phi)|^2}{r^2},$$
$$\boldsymbol{j}_{\text{inc}} = \boldsymbol{e}_z\Big(\frac{\hbar k}{m}\Big) = v\boldsymbol{e}_z.$$

Then we need to derive the relation between the cross-section of the incident and scattering. We will introduce the Differential Scattering Cross-Section.

Differential Scattering Cross-Section

Take a cube shown in Fig. 18, then one yields

$$\boldsymbol{j}_{\text{inc}}\mathrm{d}\boldsymbol{\sigma}_{\text{inc}} = v\mathrm{d}\sigma = \boldsymbol{j}_{\text{scatt}} \cdot \mathrm{d}\boldsymbol{\sigma}_{\text{scatt}} = \frac{|f(\theta,\phi)|^2}{r^2}vr^2\mathrm{d}\Omega.$$

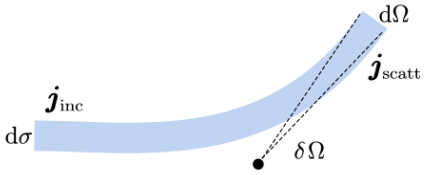


Fig. 20: Scattering cross-section.

Hence, we can define the Differential Scattering Cross-Section:

$$\sigma(\theta,\phi)=\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}=|f(\theta,\phi)|^2.$$

If $V(x)$ is a central potential, then the wavefunction is symmetric with ϕ, which then gives:

$$\Big[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\Big(r^2\frac{\partial}{\partial r}+\frac{\hbar^2 l(l+1)}{2mr^2}+V(r)\Big)\Big]\psi(r,\theta)=E\psi(r,\theta).$$

The solution of the above equation includes the radial and azimuthal parts, while the latter part is spherical harmonic function, i.e.,

$$\psi(r,\theta)=R_{nl}(r)Y_{lm}(\theta,\phi).$$

We can decompose the wavefunction according to different azimuthal quantum number "l". This is called the partial wave method.

$$\psi(r,\theta)=\sum_{l=0}^{\infty}a_l\cdot P_l(\cos\theta)\cdot R_{kl}(r)=\psi_{\text{inc}}+\psi_{\text{scatt}}.$$

For the incident wave, one has

$$\begin{aligned}e^{ikz}=e^{ikr\cos\theta}&=\sum_{l=0}^{\infty}(2l+1)i^l\cdot j_l(kr)P_l(\cos\theta)\\&\xrightarrow{kr\to\infty}\sum_{l=0}^{\infty}(2l+1)i^l\frac{1}{kr}\sin(kr-\frac{l\pi}{2})P_l(\cos\theta)\\&=\sum_{l=0}^{\infty}\frac{2l+1}{2ikr}[(-)^{l+1}e^{-ikr}+e^{ikr}]P_l(\cos\theta).\end{aligned}$$

Let

$$a_l = \frac{2l+1}{2k} i^l e^{i\delta_l},$$

where δ_l is the phase shift for the l^{th} partial wave. The total wavefunction is:

$$\begin{aligned}
\psi(r,\theta) &\overset{kr\to\infty}{\longrightarrow} \sum_{l=0}^{\infty} \frac{(-i)^l e^{-i\delta_l}}{ir}[(-)^{l+1}e^{-ikr} + e^{ikr}\cdot e^{i2\delta_l}]P_l(\cos\theta) \\
&= \sum_{l=0}^{\infty} \frac{(-i)^l e^{-i\delta_l}}{ir}[(-)^{l+1}e^{-ikr} + e^{ikr}]P_l(\cos\theta) + \\
&\qquad\qquad \sum_{l=0}^{\infty} \frac{(-i)^l e^{-i\delta_l}}{ir}(e^{i2\delta_l}-1)e^{ikr}\cdot P_l(\cos\theta) \\
&= e^{ikz} + \frac{e^{ikr}}{r}\sum_{l=0}^{\infty}\Big(\frac{2l+1}{2ik}\Big)(e^{2i\delta_l}-1)P_l(\cos\theta).
\end{aligned}$$

Then, we can obtain the scattering amplitude:

$$f(\theta,\phi) = \frac{1}{2ik}\sum_{l=0}^{\infty}\Big(\frac{2l+1}{2ik}\Big)(e^{2i\delta_l}-1)e^{ikr}P_l(\cos\theta).$$

In the above expression, when $l=0$, correspond to s-wave; when $l=1$, correspond to p-wave; when $l=2$, correspond to d-wave; when $l=3$, correspond to f-wave, etc..

The total cross section can then be derived:

$$\begin{aligned}
\sigma &= \int_\Omega |f(\theta)|^2 \mathrm{d}\Omega \\
&= \int \left|\sum_{l=0}^{\infty}\Big(\frac{2l+1}{2ik}\Big)(e^{2i\delta_l}-1)P_l(\cos\theta)\right|^2 \mathrm{d}\Omega \\
&= \Big(\frac{4\pi}{k}\Big)^2 \sum_{l=0}^{\infty}\sin^2\delta_l\Big(\frac{2l+1}{4\pi}\Big)P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{k}}) \\
&= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l = \sum_{l=0}^{\infty}\sigma_l.
\end{aligned}$$

Hard Sphere Scattering

We consider a simplified model, in which the potential is infinity inside the sphere, while is zero outside the sphere.

$$V(r) = \begin{cases} \infty, & (r<a), \\ 0, & (r>a). \end{cases}$$

(1) $ka \ll 1$:

$\lambda = 2\pi/k$ corresponds to the de Broglie wave length of the incident wave. This case means $\lambda \gg a$, corresponding to the diffraction of long wave when incidenting on a small particle.

From the above disscussion, we know that

$$\delta_l = \frac{-(ka)^{2l+1}}{(2l-1)!!(2l+1)!!},$$

where $\delta_0 = -ka$ is the minimum phase shift, and $|\delta_0| \gg |\delta_l|$. So one yields

$$f(\theta) \approx \frac{1}{k} e^{i\delta_0} P_0(\cos\theta) \sin\delta_0 \approx \frac{1}{k} \cdot 1 \cdot 1 \cdot \delta_0 = -a.$$

Therefore,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\theta)|^2 = a^2 \to \sigma = \int \mathrm{d}\Omega \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = 4\pi a^2.$$

The largest contribution comes from s-wave ($l = 0$). (In BEC, only need to consider s-wave.)

(2) $ka \gg 1$:

Now we have $\lambda \ll a$, and:

$$e^{2i\delta_l} = -e^{-[2ika - i(l+1)\pi]} \Rightarrow \delta_l = \frac{l\pi}{2} - ka.$$

When $l \ll ka$, if l increases by 1, the phase shift of the partial wave will increase $\pi/2$; when $l > ka$, the phase shift $\delta \to 0$.

So we have:

$$\sigma \approx \frac{4\pi}{k^2} \sum_{l=0}^{ka} (2l+1) \sin^2 \delta_l.$$

Optical Theorem

The optical theorem shows the relation between the total cross section and the scattering amplitude. It cannot only apply on the central potential, but also any other potential scattering problems. The optical theorem gives:

$$\boxed{\sigma = \frac{4\pi}{k} \mathrm{Im} f(0),}$$

where $f(0) = f(\theta = 0)$, shows the forward scattering. We can prove the optical theorem in the following.

Probablity flow:

$$\begin{cases} \boldsymbol{j} = \mathrm{Re}\left[\psi^*(\boldsymbol{x})\Big(-\dfrac{i\hbar\nabla}{m}\Big)\psi(\boldsymbol{x})\right], \\ \nabla\cdot\boldsymbol{j} = 0. \end{cases}$$

From Gauss theorem we know:

$$\oiint_\Sigma \boldsymbol{j}\cdot\mathrm{d}\boldsymbol{\Sigma} = \oiint \boldsymbol{j}\cdot\boldsymbol{n}r^2\mathrm{d}\Omega.$$

Since

$$\psi = \psi_{\mathrm{inc}} + \psi_{\mathrm{scatt}} = e^{i\boldsymbol{k}\cdot\boldsymbol{x}} + \frac{e^{ikr}}{r}f(\theta,\phi),$$

where $\boldsymbol{x}$ is the position vector of the investigated point, one has:

$$\boldsymbol{j} = \mathrm{Re}\left[\Big(e^{i\boldsymbol{k}\cdot\boldsymbol{x}} + \frac{e^{ikr}}{r}f(\theta,\phi)\Big)^*\Big(-\frac{i\hbar}{m}\nabla\Big)\Big(e^{i\boldsymbol{k}\cdot\boldsymbol{x}} + \frac{e^{ikr}}{r}f(\theta,\phi)\Big)\right] = \boldsymbol{j}_{\mathrm{inc}} + \boldsymbol{j}_{\mathrm{scatt}} + \boldsymbol{j}_x.$$

Where

$$\begin{cases} \boldsymbol{j}_{\mathrm{inc}} = \mathrm{Re}\left[e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\Big(-\dfrac{i\hbar}{m}\nabla\Big)(e^{i\boldsymbol{k}\cdot\boldsymbol{x}})\right] = \dfrac{h\boldsymbol{k}}{m} = \dfrac{\hbar k}{m}\boldsymbol{e}_z = v\boldsymbol{e}_z, \\ \oiint_\Sigma \boldsymbol{j}_{\mathrm{inc}}\cdot\boldsymbol{n}r^2\mathrm{d}\Omega = \displaystyle\int_V \nabla\cdot\boldsymbol{j}_{\mathrm{inc}}\mathrm{d}^3\boldsymbol{x} = 0; \quad (\boldsymbol{j}_{\mathrm{inc}} = \mathrm{const}) \end{cases}$$

$$\begin{cases} \boldsymbol{j}_{\mathrm{scatt}} = \mathrm{Re}\left[\dfrac{e^{-ikr}}{r}f^*(\theta,\phi)\Big(-\dfrac{i\hbar}{m}\nabla\Big)\Big(\dfrac{e^{ikr}}{r}f(\theta,\phi)\Big)\right] = \boldsymbol{e}_r\dfrac{\hbar k}{m}|f(\theta,\phi)|^2\dfrac{1}{r^2}, \\ \oiint_\Sigma \boldsymbol{j}_{\mathrm{scatt}}\cdot\boldsymbol{n}r^2\mathrm{d}\Omega = \oiint_\Sigma \dfrac{\hbar k}{m}|f(\theta,\phi)|^2\mathrm{d}\Omega = \oiint \dfrac{\hbar k}{m}\mathrm{d}\sigma = \dfrac{\hbar k}{m}\sigma = v\sigma; \end{cases}$$

$$\begin{aligned} \boldsymbol{j}_x &= \mathrm{Re}\left[e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\Big(-\frac{i\hbar}{m}\nabla\Big)\Big(\frac{e^{ikr}}{r}f(\theta,\phi)\Big)\right] + \mathrm{Re}\left[\frac{e^{-ikr}}{r}f^*(\theta,\phi)\Big(-\frac{i\hbar}{m}\nabla\Big)e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\right] \\ &= \frac{v}{r}\boldsymbol{e}_r[f(\theta,\phi)e^{i(kr-\boldsymbol{k}\cdot\boldsymbol{x})}] + \frac{v}{r}\boldsymbol{e}_z\left[\big(f(\theta,\phi)e^{i(kr-\boldsymbol{k}\cdot\boldsymbol{x})}\big)^*\right] \\ &= \frac{v}{r}(\boldsymbol{e}_z+\boldsymbol{e}_r)\mathrm{Re}\left[e^{i(kr-\boldsymbol{k}\cdot\boldsymbol{x})}f(\theta,\phi)\right]. \end{aligned}$$

$$\oiint_\Sigma \boldsymbol{j}_x\cdot\boldsymbol{n}r^2\mathrm{d}\Omega = vr\mathrm{Re}\int_o^{2\pi}\mathrm{d}\phi\int_0^\pi \sin\theta\mathrm{d}\theta(1+\cos\theta)e^{ikr(1-\cos\theta)}f(\theta,\phi),$$

where θ is the angle of z-axis and the radial direction. Then,

$$\begin{aligned}
&\oiint_\Sigma \boldsymbol{j}_x \cdot \boldsymbol{n} r^2 \mathrm{d}\Omega \\
&= vr\mathrm{Re}\left\{\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\Big(\frac{1}{ikr}\Big)\frac{\mathrm{d}}{\mathrm{d}\theta}[e^{ikr(1-\cos\theta)}](1+\cos\theta)f(\theta,\phi)\right\} \\
&= \frac{v}{k}\mathrm{Im}\int_0^{2\pi}\mathrm{d}\phi\left[e^{ikr(1-\cos\theta)}(1+\cos\theta)f(\theta,\phi)\right]\Big|_{\theta=0}^{\theta=2\pi} \\
&\qquad\qquad -\frac{v}{k}\mathrm{Im}\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta e^{ikr(1-\cos\theta)}\frac{\mathrm{d}}{\mathrm{d}\theta}[(1+\cos\theta)f(\theta,\phi)].
\end{aligned}$$

When $r\to\infty$, $e^{ikr(1-\cos\theta)}$ changes rapidly, except for $\theta=0$. So,

$$\begin{aligned}
&\oiint_\Sigma \boldsymbol{j}_x\cdot\boldsymbol{n}r^2\mathrm{d}\Omega = -\frac{v}{k}\mathrm{Im}\int_0^{2\pi}2f(0,\phi)\mathrm{d}\phi = -\frac{4\pi v}{k}\mathrm{Im}f(0), \\
\Longrightarrow\quad & 0 = \oiint_\Sigma \boldsymbol{j}\cdot\boldsymbol{n}r^2\mathrm{d}\Omega \\
& = \oiint_\Sigma \boldsymbol{j}_{\mathrm{inc}}\cdot\boldsymbol{n}r^2\mathrm{d}\Omega + \oiint_\Sigma \boldsymbol{j}_{\mathrm{scatt}}\boldsymbol{n}r^2\mathrm{d}\Omega + \oiint_\Sigma \boldsymbol{j}_x\boldsymbol{n}r^2\mathrm{d}\Omega \\
& = 0 + v\sigma - \frac{4\pi v}{k}\mathrm{Im}f(0), \\
\Longrightarrow\quad & \sigma = \frac{4\pi}{k}\mathrm{Im}f(0).
\end{aligned}$$

We can also derive the above results from the method of partial waves:

$$\sigma = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l.$$

So we have

$$f(\theta) = \frac{1}{k}\sum_l (2l+1)e^{i\delta_l}\sin\delta_l\cdot P_l(\cos\theta),$$

which gives

$$\begin{aligned}
f(0) &= \frac{1}{k}\sum_l (2l+1)e^{i\delta_l}\sin\delta_l \\
&= \frac{1}{k}\sum_l (2l+1)(\cos\delta_l + i\sin\delta_l)\sin\delta_l \\
&= \frac{1}{k}\sum_l (2l+1)(\cos\delta_l\sin\delta_l + i\sin^2\delta_l). \\
\Longrightarrow\quad \mathrm{Im}f(0) &= \frac{1}{k}\sum_l (2l+1)\sin^2\delta_l.
\end{aligned}$$

Therefore,

$$\sum_l (2l+1)\sin^2\delta_l = k\mathrm{Im}f(0).$$

Then one yields

$$\sigma = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l = \frac{4\pi}{k^2}\cdot k\mathrm{Im}f(0) = \frac{4\pi}{k}\mathrm{Im}f(0).$$

The above equation is the optical theorem:

$$\boxed{\sigma = \frac{4\pi}{k}\mathrm{Im}f(0).}$$

Exercises:

1. Do the proof of the optical theorem by yourself.
2. Prove the relation of the differential cross-section and the scattering amplitude.
3. Expand the plane wave e^{ikz} using the spherical harmonics.
4. Analyze the hard sphere scattering.
5. Derive three expressions of the probability current density (Re, Im, $c + c*$).
6. Dimension analysis in far field.
7. What is the physical significances of (1) b (impact parameter); (2) scattering amplitude; (3) differential cross-section of scattering?

Lecture Notes 21 Perturbation Theory: I. Nondegenerate Case

Contents

- Non-degenerate perturbation theory;
- Application: Harmonic Oscillator.

Introduction to Perturbation Theory

The Hamiltonian of the system is:

$$\hat{H} = \hat{H}^{(0)} + \lambda\delta\hat{H},$$

where $\lambda \in [0, 1]$. It is a dimensionless, natural/artificial, factor (turn-on-off parameter).

• Let $\lambda = 0$, this is the case when we do not apply the perterbation:

$$\hat{H}^{(0)}|\psi_n^0\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle,$$

where $\hat{H}^{(0)}, |\psi_n^{(0)}\rangle, E_n^{(0)}$ are non-degenerate Hamiltonian, eigenstates and eigenvalues. Index n represents the n^{th} base in the orthonormal bases of the system. Subscript 0 means it is the zero$^{\text{th}}$-order correction of the solution.

• Let $\lambda = 1$, we consider the effect of the perterbation. The prerequisite of perterbation theory is:

$$|\delta\hat{H}| \ll |\hat{H}^{(0)}|,$$

which is equivalent to

$$\begin{cases} \langle\psi_n^{(0)}|\delta\hat{H}|\psi_n^{(0)}\rangle \ll E_n^{(0)}, \\ \langle\psi_n^{(0)}|\delta\hat{H}|\psi_m^{(0)}\rangle \ll |E_n^{(0)} - E_m^{(0)}|. \end{cases}$$

We then expand the eigenstates and eigenvalue using Taylor series:

$$f(x) = f^{(0)}(x_0) + \frac{f^{(1)}(x_0)}{1!}(x - x_0) + \frac{f^{(2)}(x_0)}{2!}(x - x_0)^2 + \cdots + \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + \cdots .$$

Analysis

Now, we need to solve the eigenvalue problem:

$$\hat{H}(\lambda)|\psi_n(\lambda)\rangle = E_n(\lambda)|\psi_n(\lambda)\rangle.$$

To get $|\psi_n(\lambda)\rangle$ and $E_n(\lambda)$, we try to represent it using $\{|\psi_m^{(0)}\rangle\}$.

$$|\psi_n(\lambda)\rangle = \sum_{m=0}^{\infty} C_m(\lambda)|\psi_m^{(0)}\rangle.$$

Expanding the E_n and C_m in λ-series, we have:

$$\begin{cases} C_m(\lambda) = C_m^{(0)} + \lambda C_m^{(1)} + \lambda^2 C_m^{(2)} + \cdots, \\ E_n(\lambda) = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots. \end{cases}$$

We know that

$$C_n(\lambda) = 1 + \lambda C_n^{(1)} + \lambda^2 C_n^{(2)} + \cdots,$$

so we can let

$$C_n^{(k)} = \delta_{0k}.$$

Substitute the expansion into the eigenvalue equation, gives:

$$(\hat{H}_0 + \lambda\delta\hat{H})(\sum_{m=0}^{\infty} C_m(\lambda)|\psi_m^{(0)}\rangle) = \sum_{m=0}^{\infty}(E_n^{(0)} + \lambda E_n^{(1)} + \cdots)(C_m(\lambda)|\psi_m^{(0)}\rangle).$$

Multiplying from the left $\langle\psi_k^{(0)}|$ gives

$$\begin{aligned} l.h.s &= \langle\psi_k^{(0)}|(\hat{H}_0 + \lambda\delta\hat{H})(\sum_{m=0}^{\infty} C_m(\lambda)|\psi_m^{(0)}\rangle) \\ &= \sum_{m=0}^{\infty}(C_m^{(0)} + \lambda C_m^{(1)} + \lambda^2 C_m^{(2)} + \cdots)(E_m^{(0)}\delta_{mk} + \lambda\delta\hat{H}_{km}) \\ &= E_k^{(0)}(C_k^{(0)} + \lambda C_k^{(1)} + \lambda^2 C_k^{(0)} + \cdots) + \lambda\sum_m \delta\hat{H}_{km}(C_m^{(0)} + \lambda C_m^{(1)} + \lambda^2 C_m^{(2)} + \cdots), \\ r.h.s &= \langle\psi_k^{(0)}|\sum_{m=0}^{\infty}(E_n^{(0)} + \lambda E_n^{(1)} + \cdots)(C_m(\lambda)|\psi_m^{(0)}\rangle) \\ &= \sum_{m=0}^{\infty}(E_n^{(0)} + \lambda E_n^{(1)} + \cdots)(C_m^{(0)} + \lambda C_m^{(1)} + \lambda^2 C_m^{(2)} + \cdots)\delta_{mk} \\ &= (E_n^{(0)} + \lambda E_n^{(1)} + \cdots)(C_k^{(0)} + \lambda C_k^{(1)} + \lambda^2 C_k^{(2)} + \cdots). \end{aligned}$$

Check the terms of each orders of λ, we have:

(0) λ^0 :

$$E_k^{(0)} C_k^{(0)} = E_n^{(0)} C_k^{(0)},$$

i.e.,

$$(E_n^{(0)} - E_k^{(0)}) C_k^{(0)} = 0.$$

So we have

$$\boxed{C_k^{(0)} = \delta_{nk}.}$$

(1) λ^1 :

$$\begin{aligned} & E_n^{(0)} C_k^{(1)} + E_n^{(1)} C_k^{(0)} = C_k^{(1)} E_k^{(0)} + \sum_{m=0}^{\infty} C_m^{(0)} \delta \hat{H}_{km}, \\ \Longrightarrow \quad & E_n^{(0)} C_k^{(1)} + E_n^{(1)} \delta_{nk} = C_k^{(1)} E_k^{(0)} + \sum_{m=0}^{\infty} \delta_{nm} \delta \hat{H}_{km}, \\ \Longrightarrow \quad & E_n^{(0)} C_k^{(1)} + E_n^{(1)} \delta_{nk} = C_k^{(1)} E_k^{(0)} + \delta \hat{H}_{kn}. \end{aligned}$$

When $k = n$, we get the first-order correction of the energy:

$$E_n^{(0)} C_n^{(1)} + E_n^{(1)} \cdot 1 = C_n^{(1)} E_n^{(0)} + \delta \hat{H}_{nn},$$

which gives

$$\boxed{E_n^{(1)} = \delta \hat{H}_{nn}}.$$

When $k \neq n$, we get the first-order correction of the state:

$$E_n^{(0)} C_n^{(1)} + 0 = C_n^{(1)} E_n^{(0)} + \delta \hat{H}_{nn},$$

which gives

$$\boxed{C_k^{(1)} = \frac{\delta \hat{H}_{kn}}{E_n^{(0)} - E_k^{(0)}}.}$$

(2) λ^2 :

$$\begin{aligned} & \sum_m (C_m^{(2)} E_m^{(0)} \delta_{mk} + C_m^{(1)} \delta \hat{H}_{km}) = E_n^{(0)} C_k^{(2)} + E_n^{(1)} C_k^{(1)} + E_n^{(2)} C_k^{(2)}, \\ \Longrightarrow \quad & C_k^{(2)} E_k^{(0)} + \sum_m C_m^{(1)} \delta \hat{H}_{km} = E_n^{(0)} C_k^{(2)} + E_n^{(1)} C_n^{(1)} + E_n^{(2)} C_k^{(0)}. \end{aligned}$$

When $n = k$, we have:

$$C_n^{(2)} E_n^{(0)} + \sum_m C_m^{(1)} \delta\hat{H}_{nm} = E_n^{(0)} C_n^{(2)} + E_n^{(1)} C_n^{(1)} + E_n^{(2)}.$$

So we get the second-order correction of the energy:

$$E_n^{(2)} = \sum_m C_m^{(1)} \delta\hat{H}_{nm} - E_n^{(1)} C_n^{(1)} = \sum_{m \neq n} C_m^{(1)} \delta\hat{H}_{nm} = \sum_{m \neq n} \frac{|\delta\hat{H}_{nm}|^2}{E_n^{(0)} - E_m^{(0)}}.$$

When $n \neq k$, we have:

$$C_k^{(2)} E_k^{(0)} + \sum_m C_m^{(1)} \delta\hat{H}_{km} = E_n^{(0)} C_k^{(2)} + \delta H_{nn} C_k^{(1)} + 0.$$

So we get the second-order correction of the state:

$$\begin{aligned} C_k^{(2)} &= \frac{1}{E_n^{(0)} - E_k^{(0)}} \left[\sum_{m \neq n} C_m^{(1)} \delta\hat{H}_{km} - \delta\hat{H}_{nn} C_k^{(1)} \right] \\ &= \frac{1}{E_n^{(0)} - E_k^{(0)}} \left[\sum_{m \neq n} \frac{\delta\hat{H}_{mn} \delta\hat{H}_{km}}{E_n^{(0)} - E_m^{(0)}} - \delta\hat{H}_{nn} \frac{\delta\hat{H}_{kn}}{E_n^{(0)} - E_k^{(0)}} \right]. \end{aligned}$$

We only keep the correction of energy to the second order and the correction of state to first order, then

$$\begin{cases} E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} = E_n^{(0)} + \delta\hat{H}_{nn} + \sum_{m \neq n} \dfrac{|\delta\hat{H}_{nk}|^2}{E_n^{(2)} - E_k^{(2)}}. \\ |\psi_n\rangle = |\psi_n^{(0)}\rangle + \sum_{k \neq n} \dfrac{\delta\hat{H}_{kn}}{E_n^{(0)} - E_k^{(0)}} |\psi_k^{(0)}\rangle. \end{cases}$$

Application

Take harmonic oscillator as an example. The zeroth-order Hamiltonian, energy and eigenstates are:

$$\begin{cases} \hat{H}^{(0)} = \hbar\omega(\hat{a}\hat{a}^\dagger + \dfrac{1}{2}), \\ E_n^{(0)} = \hbar\omega(n + \dfrac{1}{2}), \\ |\psi_n^{(0)}\rangle = |n\rangle. \end{cases}$$

Define the ladder operators (annihilation/creation operators):

$$\begin{cases} \hat{a} = \sqrt{\dfrac{m\omega}{2\hbar}}\hat{x} + \dfrac{i}{\sqrt{2m\hbar\omega}}\hat{p}, \\ \hat{a}^\dagger = \sqrt{\dfrac{m\omega}{2\hbar}}\hat{x} - \dfrac{i}{\sqrt{2m\hbar\omega}}\hat{p}, \end{cases}$$

In the following, we use the occupation number state representation. Review some properties:

$$\begin{cases} \hat{a}^\dagger\hat{a}|n\rangle = \hat{N}|n\rangle = n|n\rangle, \\ \hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \\ \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \\ \langle n|\hat{a}|n\rangle = \langle n|\hat{a}^\dagger|n\rangle = 0. \end{cases}$$

Consider the perturbation like:

$$\delta\hat{H} = -q\mathcal{E}\hat{x} = -\alpha\hbar\omega(\hat{a} + \hat{a}^\dagger),$$

where $\alpha = \sqrt{m\omega/2\hbar}x_0,\ x_0 = q\mathcal{E}/m\omega^2$.

Using the perturbation theory, we have:

(1) The first-order correction of energy:

$$E_n^{(1)} = \delta\hat{H}_{nn} = \langle\psi_n^{(0)}|\delta\hat{H}|\psi_n^{(0)}\rangle = \langle n|(-\alpha\hbar\omega)(\hat{a} + \hat{a}^\dagger)|n\rangle = 0.$$

(2) The first-order correction of state:

$$\delta\hat{H}_{kn} = (-\alpha\hbar\omega)(\sqrt{n}\delta_{n-1,k} + \sqrt{n+1}\delta_{n+1,k}),$$

So we have:

$$\begin{aligned} |n'\rangle &= |n\rangle + \sum_{k\neq n}\frac{\delta\hat{H}_{kn}}{E_n^{(0)} - E_k^{(0)}}|k\rangle \\ &= |n\rangle + \frac{\delta\hat{H}_{n-1,n}}{E_n^{(0)} - E_{n-1}^{(0)}}|n-1\rangle + \frac{\delta\hat{H}_{n+1,n}}{E_n^{(0)} - E_{n+1}^{(0)}}|n+1\rangle \\ &= |n\rangle - \frac{\alpha\hbar\omega\sqrt{n}}{E_n^{(0)} - E_{n-1}^{(0)}}|n-1\rangle - \frac{\alpha\hbar\omega\sqrt{n+1}}{E_n^{(0)} - E_{n+1}^{(0)}}|n+1\rangle \\ &= |n\rangle - \alpha\sqrt{n}|n-1\rangle + \alpha\sqrt{n+1}|n+1\rangle. \end{aligned}$$

(3) The second-order correction of energy:

$$E_n^{(2)} = \sum_{k\neq n} \frac{|\delta\hat{H}_{nk}|^2}{E_n^{(2)} - E_k^{(2)}} = \sum_{k\neq n} \frac{|\delta\hat{H}_{nk}|^2}{\hbar\omega(n-k)},$$

so,

$$E_n^{(2)} = \frac{(-\alpha\hbar\omega\sqrt{n})^2}{\hbar\omega} - \frac{(-\alpha\hbar\omega\sqrt{n+1})^2}{\hbar\omega} = -\alpha^2\hbar\omega.$$

Based on the first-order correction of state, we have:

$$\begin{aligned}\langle\hat{x}\rangle &= \langle\psi_n|\hat{x}|\psi_n\rangle \\ &= (\langle n| - \alpha\sqrt{n}\langle n-1| + \alpha\sqrt{n+1}\langle n+1|)(\hat{a}+\hat{a}^\dagger) \\ &\qquad \sqrt{\frac{\hbar}{2m\omega}}(|n\rangle - \alpha\sqrt{n}|n-1\rangle + \alpha\sqrt{n+1}|n+1\rangle) = \frac{q\mathcal{E}}{m\omega^2}.\end{aligned}$$

Polarization strength of the atom is:

$$P = 2|q|\langle\hat{x}\rangle = 2q^2\frac{\mathcal{E}}{m\omega^2} = \chi\mathcal{E},$$

where $\chi = 2q^2/m\omega^2$, is the polarization susceptibility.

• Summary:

$$\begin{cases} E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} = \hbar\omega\Big(n+\dfrac{1}{2}\Big) - \dfrac{q^2\mathcal{E}^2}{2m\omega^2}, \\ |\psi_n\rangle = |n\rangle + \alpha(\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle), \\ \hat{H} = \hat{H}_0 + \delta\hat{H} = \hbar\Big(\hat{a}^\dagger\hat{a} + \dfrac{1}{2}\Big) - \hbar\omega\alpha(\hat{a}+\hat{a}^\dagger) = \hbar\omega\Big[(\hat{a}^\dagger-\alpha)(\hat{a}-\alpha) + \dfrac{1}{2}(1-\alpha^2)\Big]. \end{cases}$$

Exercises:

1. If the perturbation in the harmonic oscillator is proportional to $\hat{x}^4$, try to give the first-order correction of the energy.

2. Rederive the perturbation terms of the eigenvalue (up to the 2nd-order correction) and eigenstates (up to the 1st-order correction).

Lecture Notes 22 Perturbation Theory: II. Degenerate Case

Contents

- Degenerate Perturbation Theory;
- Application: Stark Effect.

1. Basics:

The Hamiltonian of the system is:

$$\hat{H} = \hat{H}^{(0)} + \lambda\delta\hat{H}, \quad (\lambda \in [0,1]).$$

In the degenerate case, the solution to the unperturbed eigenvalue problem is:

$$\hat{H}^{(0)}|n\nu\rangle = E_n^{(0)}|n\nu\rangle, \quad (\nu = 1, \cdots, \nu_n),$$

where ν_n is the degeneracy, and we have:

$$\begin{cases} \lambda < 1 \to \lambda^k\text{-series} \begin{cases} \lambda : \text{dimensionless, small} \\ \lambda : \text{natural/ artificial} \end{cases} \\ |\lambda\delta\hat{H}| \ll |\hat{H}^{(0)}|. \end{cases}$$

In the degenerate case, the bases also satisfy the orthonormality and completeness:

$$\begin{cases} \langle n'\nu'|n\nu\rangle = \delta_{nn'}\delta_{\nu\nu'}, \\ \sum\limits_{n\nu} |n\nu\rangle\langle n\nu| = \mathbb{1}. \end{cases}$$

2. Analysis

We apply the perturbation and have:

$$\hat{H}|\psi_k\rangle = E_k|\psi_k\rangle.$$

where

$$|\psi_k\rangle = \sum_{m\mu} C_{m\mu}|m\mu\rangle, \quad C_{m\mu} = \langle m\mu|\psi_k\rangle.$$

Expand the energy and coefficient in λ-series:

$$\begin{cases} E_k = \lambda^0 E_k^{(0)} + \lambda^1 E_k^{(1)} + \lambda^2 E_k^{(2)} + \cdots, \\ C_{m\mu} = \lambda^0 C_{m\mu}^{(0)} + \lambda^1 C_{m\mu}^{(1)} + \lambda^2 C_{m\mu}^{(2)} + \cdots. \end{cases}$$

Multiplying $\langle m\mu|$ from the left to both sides of the equation, gives

$$\begin{aligned} l.h.s = \langle m\mu|(\hat{H}^{(0)} + \lambda\delta\hat{H})|\psi_k\rangle &= E_m^{(0)}\langle m\mu|\psi_k\rangle + \lambda\langle m\mu|\delta\hat{H}|\psi_k\rangle \\ &= E_m^{(0)} C_{m\mu} + \sum_{n\nu}\langle m\mu|\lambda\delta\hat{H}|n\nu\rangle\langle n\nu|\psi_k\rangle \\ &= E_m^{(0)} C_{m\mu} + \sum_{n\nu}\lambda\delta\hat{H}_{m\mu,n\nu} C_{n\nu} \\ &= E_m^{(0)}(C_{m\mu}^{(0)} + \lambda C_{m\mu}^{(1)} + \cdots) + \sum_{n\nu}\lambda\delta\hat{H}_{m\mu,n\nu}(C_{n\nu}^{(0)} + \lambda C_{n\nu}^{(1)} + \cdots) \\ &= E_m^{(0)} C_{m\mu}^{(0)} + \lambda(E_m^{(0)} C_{m\mu}^{(1)} + \sum_{n\nu}\delta\hat{H}_{m\mu,n\nu} C_{n\nu}^{(0)}) + O(\lambda^2), \end{aligned}$$

$$\begin{aligned} r.h.s = E_k\langle m\mu|\psi_k\rangle = E_k C_{m\mu} &= (\lambda^0 E_k^{(0)} + \lambda^1 E_k^{(1)} + \cdots)(\lambda^0 C_{m\mu}^{(0)} + \lambda^1 C_{m\mu}^{(1)} + \cdots) \\ &= E_k^{(0)} C_{m\mu}^{(0)} + \lambda(E_k^{(1)} C_{m\mu}^{(0)} + E_k^{(0)} C_{m\mu}^{(1)}) + O(\lambda^2). \end{aligned}$$

Therefore, one has:

(0) λ^0:

$$\begin{aligned} & E_k^{(0)} C_{m\mu}^{(0)} = E_m^{(0)} C_{m\mu}^{(0)}, \\ \Longrightarrow \quad & (E_m^{(0)} - E_k^{(0)}) C_{m\mu}^{(0)} = 0. \end{aligned}$$

Hence,

$$\boxed{C_{m\mu}^{(0))} = a_\mu \delta_{km}.}$$

(1) λ^1:

$$E_k^{(1)} C_{m\mu}^{(0)} + E_k^{(0)} C_{m\mu}^{(1)} = E_m^{(0)} C_{k\mu}^{(1)} + \sum_{n\nu}\delta\hat{H}_{m\mu,n\nu} C_{n\nu}^{(0)}.$$

Substitute the zeroth-order coefficient into the equation, gives

$$E_k^{(1)} a_\mu \delta_{km} + E_k^{(0)} C_{m\mu}^{(1)} = E_m^{(0)} C_{k\mu}^{(1)} + \sum_{n\nu}\delta\hat{H}_{m\mu,n\nu} a_\nu \delta_{kn}.$$

When $m = k$, one has

$$\begin{aligned} & E_k^{(1)} a_\mu + E_k^{(0)} C_{k\mu}^{(1)} = E_k^{(0)} C_{k\mu}^{(1)} + \sum_\nu \delta\hat{H}_{k\mu,k\nu} a_\nu \\ \rightarrow \quad & E_k^{(1)} a_\mu = \sum_\nu \delta\hat{H}_{k\mu,k\nu} a_\nu \\ \rightarrow \quad & \sum_\nu (\delta\hat{H}_{\mu\nu} - E_k^{(1)}\delta_{\mu\nu}) a_\nu = 0, \end{aligned}$$

where a simplified matrix element notation $\delta\hat{H}_{\mu\nu} = \delta\hat{H}_{k\mu,k\nu}$ is adopted.

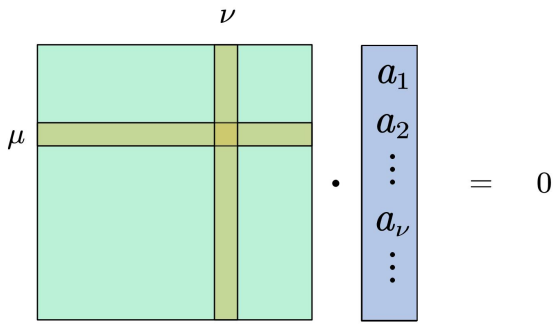


Fig. 21: Matrix representation of the secular equation.

We can write it out in form of the matrix:

$$\begin{pmatrix} \delta\hat{H}_{11} - E_k^{(1)} & \delta\hat{H}_{12} & \delta\hat{H}_{13} & \cdots \\ \vdots & \delta\hat{H}_{22} - E_k^{(1)} & \delta\hat{H}_{23} & \cdots \\ & \vdots & \delta\hat{H}_{33} - E_k^{(1)} & \cdots \\ & & \vdots & \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = 0.$$

Conditions for the existence of solutions of the secular equations is:

$$\det |\delta\hat{H}_{\mu\nu} - E_k^{(1)}\delta_{\mu\nu}| = 0.$$

This is called secular equation (久期方程). We get α_k solutions $E_{k\alpha}^{(1)} \quad (\alpha = 1, \cdots, \alpha_k)$, and α_k sets of coefficients $a_{\nu\alpha} \quad (\nu = 1, \cdots, \nu_k)$. There are three cases:

(1) $\alpha_k = 1$, (no elimination of degeneracy);

(2) $\alpha_k = \nu_k$, (degeneracy eliminated completely);

(3) $1 < \alpha_k < \nu_k$. (degeneracy eliminated partially).

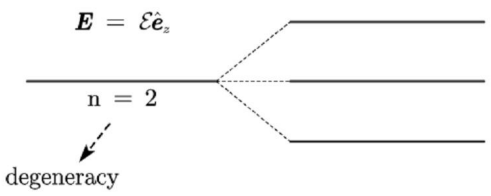


Fig. 22: Stark effect of Hydrogen atom.

We keep the correction of energy up to the first-order, and the correction of state up to the zeroth-order, then:

$$\begin{cases} |\psi_{k\alpha}\rangle = \sum_{\mu} a_{\mu\alpha}|k\mu\rangle. \\ E_k^{(1)} = E_{k\alpha}^{(1)}. \end{cases}$$

3. Stark Effect:

We take the stark effect of the hydrogen atom as an example. For the $n = 2$ energy level (the degeneracy is 4):

$$\begin{cases} |n=2, l=0, m_l=0\rangle = |200\rangle, & (2s \text{ state}) \\ |n=2, l=1, m_l=-1\rangle = |21-1\rangle, & (2p_{-1} \text{ state}) \\ |n=2, l=1, m_l=0\rangle = |210\rangle, & (2p_0 \text{ state}) \\ |n=2, l=1, m_l=1\rangle = |211\rangle. & (2p_1 \text{ state}). \end{cases}$$

The energy of the unperturbed state is:

$$E_n = -\frac{e^2}{2a_0}\frac{1}{n^2} = -13.6\text{eV} \times \frac{1}{n^2} \xlongequal{n=2} -3.4\text{eV}.$$

The four eigenstates are simplified by the following:

$$\begin{aligned} |1\rangle &= |200\rangle, \\ |2\rangle &= |210\rangle, \\ |3\rangle &= |211\rangle, \\ |4\rangle &= |21-1\rangle. \end{aligned}$$

The eigenvalue equation of the unperturbed system is:

$$\hat{H}^{(0)}|2lm\rangle = E_2^{(0)}|2lm\rangle, \quad (l = 0, 1;\ m = 0, \pm 1)$$

The perturbation Hamiltonian in the spherical coordinates is:

$$\lambda\delta\hat{H} = e\mathcal{E}z = e\mathcal{E}r\cos\theta = \frac{e\mathcal{E}a_0}{e^2/a_0} \cdot \frac{e^2}{a_0^2} r\cos\theta,$$

where a_0 is the Bohr radius, and we can take the turn-on-off factor as:

$$\lambda = \frac{e\mathcal{E}a_0}{e^2/a_0} = \frac{W_{\text{ext}}}{W_{\text{col}}},$$

which is a dimensionless parameter. We assume that the external field is weak, so $\lambda \ll 1$, and

$$\delta\hat{H} = \frac{a^2}{a_0^2} r\cos\theta,$$

which is the work done by the Coloumb's force in the range $z = r\cos\theta$. As we know:

$$\delta\hat{H}_{\mu\nu} = \delta\hat{H}_{k\mu,k\nu}, \quad (k = 2;\ \mu, \nu = 1, 2, 3, 4),$$

so we need to calculate the elements of a 4×4 matrix. To reduce our calculations, we can use the selection rule to find out all the "zero matrix element".

(1) The selection rule for m:

$$[\hat{L}_i, \hat{x}_j] = i\hbar\epsilon_{ijk}\hat{x}_k \Rightarrow [\hat{L}_z, \hat{z}] = 0,$$

$$\Longrightarrow \quad \langle l'm'|\hat{z}|lm\rangle = \delta_{mm'}.$$

So we have the selection rule for m:

$$\boxed{\Delta m = 0.}$$

(2) The selection rule for l:

In $\boldsymbol{x}$-representation, we have:

$$|lm\rangle = Y_{lm_l}(\theta, \phi),$$

which has the relation:

$$\cos\theta Y_{lm_l}(\theta,\phi) \sim aY_{l+1,m_l}(\theta,\phi) + bY_{l-1,m_l}(\theta,\phi) = a|l+1,m_l\rangle + b|l-1,m_l\rangle.$$

So,

$$\langle lm|\delta\hat{H}|lm\rangle \sim \delta_{l\pm1,l'}.$$

That is to say, the selection rule for l is:

$$\boxed{\Delta l = l - l' = \pm 1.}$$

According to the above discussioins, one finds that the only non-zero matrix element needed to be calculated is the transition of $|200\rangle \leftrightarrow |210\rangle$:

$$\begin{aligned}
\langle 1|\lambda\delta\hat{H}|2\rangle &= \langle 2|\lambda\delta\hat{H}|1\rangle \\
&= \langle 200|\lambda\delta\hat{H}|210\rangle \\
&= \int \psi^*_{200}(\theta,\phi)(\lambda\delta\hat{H})\psi_{210}(\theta,\phi)r^2\mathrm{d}r\sin\theta\mathrm{d}\theta\mathrm{d}\phi \\
&= -3ea_0\mathcal{E}.
\end{aligned}$$

Then we have the secular equation:

$$\begin{vmatrix}
-E_2^{(1)} & -3ea_0\mathcal{E} & 0 & 0 \\
-3ea_0\mathcal{E} & -E_2^{(1)} & 0 & 0 \\
0 & 0 & -E_2^{(1)} & 0 \\
0 & 0 & 0 & -E_2^{(1)}
\end{vmatrix} = 0.$$

Solving the secular equation gives $E_2^{(1)} = 0, \pm 3ea_0\mathcal{E}$, while the corresponding states are:

$$|\psi_k\rangle = \begin{cases}
|211\rangle, |21-1\rangle, & (\Delta E = 0) \\
\dfrac{1}{\sqrt{2}}(|200\rangle + |210\rangle), & (\Delta E = -3ea_0\mathcal{E}) \\
\dfrac{1}{\sqrt{2}}(|200\rangle - |210\rangle), & (\Delta E = 3ea_0\mathcal{E}).
\end{cases}$$

We find that the degeneracy is partially eliminated, while for $\Delta E = 0$ there are still 2-degeneracy remained.

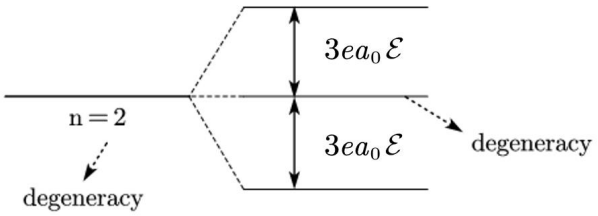


Fig. 23: Stark effect of Hydrogen atom.

Exercises:

1. Try to derive the first-order correction of the state in degenerate perturbation theory.

2. Derive $\langle 1|\lambda\delta\hat{H}|2\rangle = -3ea_0\mathcal{E}$.

3. Derive the selection rule for m and l.

4. Compare the degenerate and non-degenerate perturbation theory and tell the differences.

5. Try to discuss the physical significances of the small parameter λ in degenerate/non-degenerate perturbation theories.

6. Besides the Stark effect of Hydrogen atom, try to solve the case for another atom.

Lecture Notes 23 Charged Particles in EM Field

Contents

- Classical Electromagnetic Theory;
- Non-relativistic QM Theory ;
- Relativistic QM Theory.

1. Classical Electromagnetic Theory:

In classical mechanics, we have:

$$\hat{H} = \frac{1}{2m}(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A})^2 + q\phi. \qquad \begin{cases} \boldsymbol{p}, & \text{(canonical momentum)} \\ \boldsymbol{x}, & \text{(canonical position)} \\ \boldsymbol{A} = \boldsymbol{A}(\boldsymbol{x}, t), & \text{(vector potential)} \\ \phi = \phi(\boldsymbol{x}, t). & \text{(scalar potential)} \end{cases}$$

According to the canonical equations, we can derive the Newton-Lorentz equation in EM field:

$$\begin{cases} \dfrac{\partial \hat{H}}{\partial p_\alpha} = \dot{x}_\alpha, \\ \dfrac{\partial \hat{H}}{\partial x_\alpha} = -\dot{p}_\alpha. \end{cases} \Rightarrow \begin{cases} m\ddot{\boldsymbol{x}} = q\Big(\boldsymbol{E} + \dfrac{\boldsymbol{v}}{c} \times \boldsymbol{B}\Big), \\ \boldsymbol{E} = -\nabla\phi - \dfrac{1}{c}\dfrac{\partial \boldsymbol{A}}{\partial t}, \quad \boldsymbol{B} = \nabla \times \boldsymbol{A}. \end{cases}$$

The following gives the procedure of deriving Newton-Lorentz's equation.

$$\Longrightarrow \quad \begin{cases} \dot{x}_i = \dfrac{\partial \hat{H}}{\partial p_i} = \dfrac{1}{m}\Big(p_i - \dfrac{q}{c}A_i\Big) = v_i, \\ \dot{p}_i = -\dfrac{\partial \hat{H}}{\partial x_i} = -\dfrac{1}{m}\Big(p_j - \dfrac{q}{c}A_j\Big)\Big(-\dfrac{q}{c}\partial_i A_j\Big) - q\partial_i\phi = -q\partial_i\phi + \dfrac{q}{c}v_i\partial_i A_j, \end{cases}$$

$$\Longrightarrow \quad \begin{cases} \ddot{x}_i = \dfrac{1}{m}\Big(\dot{p}_i - \dfrac{q}{c}\dot{A}_i\Big), \\ \dot{A}_i = \dfrac{\mathrm{d}}{\mathrm{d}t}A_i = \dfrac{\partial A_i}{\partial t} + \dfrac{\partial A_i}{\partial x_j}\dfrac{\mathrm{d}x_j}{\mathrm{d}t} = \partial_t A_i + v_j\partial_j A_i, \end{cases}$$

$$\begin{aligned}\Longrightarrow \quad m\ddot{x}_i &= \dot{p}_i - \frac{q}{c}(\partial_t A_i + v_j \partial_j A_i) \\ &= -q\partial_i \phi + \frac{q}{c} v_j \partial_i A_j - \frac{q}{c}\partial_t A_i - \frac{q}{c} v_j \partial_j A_i \\ &= q(-\partial_i \phi - \frac{1}{c}\partial_t A_i) + \frac{q}{c} v_j (\partial_i A_j - \partial_j A_i) \\ &= qE_i + q\Big(\frac{\boldsymbol{v}\times \boldsymbol{B}}{c}\Big)_i .\end{aligned}$$

where $\partial_i = \partial/\partial x_i,\ \partial_t = \partial/\partial t$.

2. Non-relativistic QM Theory (spinless)

$$\begin{cases} \hat{H} = \dfrac{1}{2m}\Big[\hat{\boldsymbol{p}} - \dfrac{q}{c}\hat{\boldsymbol{A}}(\boldsymbol{x}, t)\Big]^2 + q\phi(\boldsymbol{x}, t), \\ [\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}, \quad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0. \end{cases}$$

The Hamiltonian is:

$$\hat{H} = \frac{1}{2m}(\hat{\boldsymbol{p}}^2 - \frac{q}{c}\hat{\boldsymbol{p}}\cdot\boldsymbol{A} - \frac{q}{c}\boldsymbol{A}\cdot\hat{\boldsymbol{p}} + \frac{q^2}{c^2}\boldsymbol{A}^2) + q\phi.$$

Note that:

$$[\hat{p}_i, A_j] = [\hat{p}_i, \hat{x}_\alpha]\partial_\alpha A_j = -i\hbar\delta_{i\alpha}\partial_\alpha A_j = -i\hbar\partial_i A_j.$$

But if we take Coulumb gauge, i.e., $\nabla\cdot\boldsymbol{A} = 0$, so the momentum operator commutes with the vector potential (for the same component). Since:

$$\Big|\frac{q^2}{c^2}\boldsymbol{A}^2\Big| \ll \Big|\frac{q}{c}\boldsymbol{A}\cdot\boldsymbol{p}\Big|,$$

it can be ignored. Also, we take radiation gauge, which means $\phi = 0$, so the Hamiltonian is:

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{q}{mc}\boldsymbol{A}\cdot\hat{\boldsymbol{p}}.$$

Since normally, the atom is small (compared with the wavelength of EM field), so the magnetic field can be taken as a constant, then the vector potential is:

$$\boldsymbol{A} = \frac{1}{2}\boldsymbol{B}\times\hat{\boldsymbol{x}}.$$

We can verify this relation by substituting the above expression into $\boldsymbol{\nabla}\times\boldsymbol{A}$ and $\boldsymbol{\nabla}\cdot\boldsymbol{A}$ to see if it matches $\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$ and Coloumb gauge $\boldsymbol{\nabla}\cdot\boldsymbol{A} = 0$.

(1) $\boldsymbol{\nabla}\times\boldsymbol{A}$:

$$\begin{aligned}(\boldsymbol{\nabla}\times\boldsymbol{A})_i &= \frac{1}{2}\epsilon_{ijk}\partial_j\epsilon_{klm}B_l x_m \\ &= \frac{1}{2}(\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl})\partial_j B_l x_m \\ &= \frac{1}{2}(\partial_j B_i x_j - \partial_j B_j x_i) \\ &= \frac{1}{2}(\delta_{jj}B_i - B_j\delta_{ij}) = B_i,\end{aligned}$$

i.e.,

$$\boldsymbol{\nabla}\times\boldsymbol{A}=\boldsymbol{B}.$$

(2) $\boldsymbol{\nabla}\cdot\boldsymbol{A}$:

$$\begin{aligned}\nabla\cdot\boldsymbol{A} &= \frac{1}{2}\partial_i\epsilon_{ijk}\frac{1}{2}B_j x_k \\ &= \delta_{ik}\epsilon_{ijk}\frac{1}{2}B_j = 0,\end{aligned}$$

i.e.,

$$\boldsymbol{\nabla}\cdot\boldsymbol{A}=0.$$

Therefore, one yields $\boldsymbol{A}=\frac{1}{2}\boldsymbol{B}\times\boldsymbol{x}$.

The interaction Hamiltonian is:

$$\begin{aligned}\hat{H}_{\mathrm{M}} &= -\frac{q}{mc}\boldsymbol{A}\cdot\hat{\boldsymbol{p}} \\ &= -\frac{q}{2mc}(\boldsymbol{B}\times\hat{\boldsymbol{x}})\cdot\hat{\boldsymbol{p}} \\ &= -\frac{q}{2mc}(\hat{\boldsymbol{x}}\times\hat{\boldsymbol{p}})\cdot\boldsymbol{B} \\ &= -\hat{\boldsymbol{\mu}}_L\cdot\boldsymbol{B},\end{aligned}$$

where

$$\hat{\boldsymbol{\mu}}_L=\frac{q}{2mc}\hat{\boldsymbol{L}}$$

is the orbital magnetic moment.

Consider the electron interacts with the magnetic field, we have:

$$\begin{aligned}\boldsymbol{\mu}_L &= \frac{q}{2mc}\hat{\boldsymbol{L}} \\ &\xrightarrow{q=-e} -\frac{e}{2mc}\hat{\boldsymbol{L}} \\ &= -\frac{e\hbar}{2mc}(\hat{\boldsymbol{L}}/\hbar) \\ &= -\mu_{\mathrm{B}}(\hat{\boldsymbol{L}}/\hbar),\end{aligned}$$

where:

$$\boxed{\mu_{\mathrm{B}} = \frac{e\hbar}{2mc}}$$

is Bhor's magnetom. Therefore the interaction Hamiltonian is:

$$\hat{H}_{\mathrm{M}} = \mu_{\mathrm{B}} B(\hat{L}_z/\hbar).$$

The following gives the order of the magnitude analysis:

(1) Electric-dipole interaction vs. Magnetic-dipole interaction:

$$\begin{cases} \hat{H}_{\mathrm{E}} = -\hat{\boldsymbol{d}} \cdot \boldsymbol{E} = ezE, \\ \hat{H}_{\mathrm{M}} = \mu_{\mathrm{B}} B(\hat{L}_z/\hbar) \sim \mu_{\mathrm{B}} B. \end{cases}$$

If $|E| \sim |B|$, we have:

$$\frac{|\hat{H}_{\mathrm{M}}|}{|\hat{H}_{\mathrm{E}}|} = \frac{\mu_{\mathrm{B}}}{ez} \sim \frac{\hbar}{mc}\frac{1}{z} \sim \frac{\lambda\!\!\!^{-}}{a_0} = \frac{1}{137} = \alpha,$$

where $\lambda\!\!\!^{-} = \hbar/mc$ is the reduced Compton wavelength, $\alpha = e^2/\hbar c = 1/137$, is the fine structure constant.

(2) Analysis of the second order terms: $(a_0 p \sim \hbar \Rightarrow p \sim \hbar/a_0)$

$$\frac{q^2}{c^2}\boldsymbol{A}^2 \sim \frac{q^2}{c^2}(\boldsymbol{B} \times \hat{\boldsymbol{x}})^2 \sim \frac{q^2}{c^2}B^2 r^2 \sim \frac{e^2}{c^2}B^2 a_0^2,$$

$$\frac{|\frac{q^2}{c^2}\boldsymbol{A}^2|}{|\frac{q}{c}\hat{\boldsymbol{p}} \cdot \boldsymbol{A}|} = \frac{|\frac{e^2}{c^2}B^2 a_0^2|}{\frac{e}{c}Ba_0 p} \sim \frac{e^2}{\hbar c}\frac{Ba_0^2}{e} \sim \alpha \cdot \frac{B}{e/a_0^2} \ll \alpha = \frac{1}{137}.$$

So we can just ignore the second order terms.

(3) Orbital magnetic moment vs. intrinsic magnetic moment

$$\begin{cases} \hat{\boldsymbol{\mu}}_L = \dfrac{e}{2mc}\hat{\boldsymbol{L}} = g_L \mu_{\mathrm{B}} \hat{\boldsymbol{L}}/\hbar, \\ \hat{\boldsymbol{\mu}}_S = \dfrac{e}{mc}\hat{\boldsymbol{L}} = g_S \mu_{\mathrm{B}} \hat{\boldsymbol{L}}/\hbar, \end{cases}$$

where g is the Landé-factor, and $g_L \approxeq 1, g_S \approxeq 2$.

3. Relativistic QM Theory (Spin)

To derive the form in Relativistic QM, we need three steps:

(1) From scalar to spinor wave functions:

$$\hat{H} = \frac{\boldsymbol{p}^2}{2m} \cdot \mathbb{1}_2 = \frac{1}{2m}(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}})^2.$$

We use the properties of Pauli matrix here:

$$(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{A}})(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{B}}) = \hat{\boldsymbol{A}} \cdot \hat{\boldsymbol{B}} + i\hat{\boldsymbol{\sigma}} \cdot (\hat{\boldsymbol{A}} \cdot \hat{\boldsymbol{B}}) \quad \rightarrow \quad (\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}})^2 = \hat{\boldsymbol{p}}^2 \cdot \mathbb{1}_2.$$

(2) From free particles to particles in EM field:

When the particle is in the EM field, the canonical momentum becomes:

$$\hat{\boldsymbol{p}} \quad \rightarrow \quad \hat{\boldsymbol{\pi}} = \hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}.$$

Then the Hamiltonian is:

$$\hat{H} = \frac{1}{2m}(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{\pi}})^2 = \frac{1}{2m}\left[\hat{\boldsymbol{\sigma}} \cdot \left(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}\right)\right]^2.$$

(3) Expand the Hamiltonian, i.e.,

$$\hat{H} = \frac{1}{2m}(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{\pi}})^2 = \frac{1}{2m}\hat{\boldsymbol{\pi}}^2 + \frac{i}{2m}\hat{\boldsymbol{\sigma}} \cdot (\hat{\boldsymbol{\pi}} \times \hat{\boldsymbol{\pi}}).$$

The first term is:

$$\frac{1}{2m}\hat{\boldsymbol{\pi}}^2 = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{e^2}{r} - \frac{q}{mc}\boldsymbol{A} \cdot \hat{\boldsymbol{p}} = \hat{H}^{(0)} + \hat{H}_{\mathrm{MNR}},$$

where:

$$\begin{cases} \hat{H}^{(0)} = \dfrac{\boldsymbol{p}^2}{2m} - \dfrac{e^2}{r}, & \text{(free Hamiltonian)} \\ \hat{H}_{\mathrm{MNR}} = -\boldsymbol{\mu_L} \cdot \boldsymbol{B} = -\mu_{\mathrm{B}}\hat{\boldsymbol{L}}\hbar. & \text{(contribution due to orbital magnetic moment)} \end{cases}$$

The second term is:

$$\begin{aligned}(\hat{\boldsymbol{\pi}}\times\hat{\boldsymbol{\pi}})_i &= \epsilon_{ijk}\hat{\pi}_j\hat{\pi}_k = \frac{1}{2}\epsilon_{ijk}\hat{\pi}_j\hat{\pi}_k - \frac{1}{2}\epsilon_{ijk}\hat{\pi}_k\hat{\pi}_j \\ &= \frac{1}{2}\epsilon_{ijk}[\hat{\pi}_j,\hat{\pi}_k] \\ &= \frac{1}{2}\epsilon_{ijk}\Big(\frac{i\hbar q}{c}\Big)(\partial_j A_k - \partial_k A_j) \\ &= \frac{i\hbar q}{2c}\epsilon_{ijk}(\partial_j A_k - \partial_k A_j) \\ &= \frac{i\hbar q}{c}\epsilon_{ijk}\partial_j A_k = \frac{i\hbar q}{c}B_i.\end{aligned}$$

So we have (note that $\hat{\boldsymbol{S}} = \dfrac{\hbar}{2}\hat{\boldsymbol{\sigma}}$)

$$\hat{H}_{\mathrm{MR}} = \frac{i}{2m}\hat{\boldsymbol{\sigma}}\cdot(\hat{\boldsymbol{\pi}}\times\hat{\boldsymbol{\pi}}) = \frac{i}{2m}\hat{\boldsymbol{\sigma}}\cdot\Big(\frac{i\hbar q}{c}\boldsymbol{B}\Big) = -\frac{\hbar q}{2mc}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B} = -\frac{q}{mc}\hat{\boldsymbol{S}}\cdot\boldsymbol{B}.$$

Therefore, the total interaction Hamiltonian is:

$$\hat{H}_{\mathrm{M}} = \hat{H}_{\mathrm{MNR}} + \mathrm{H}_{\mathrm{MR}} = -\frac{q}{2mc}\hat{\boldsymbol{L}}\cdot\boldsymbol{B} - \frac{q}{mc}\hat{\boldsymbol{S}}\cdot\boldsymbol{B} = \mu_{\mathrm{B}}B(\hat{L}_z + 2\hat{S}_z)/\hbar.$$

Exercises:

1. Try to prove the commutation relations of kinetic momentum $\hat{\pi}$:

$$[\hat{\pi}_i,\hat{\pi}_j] = \frac{iq\hbar}{c}(\partial_i A_j - \partial_j A_i) \leftrightarrow \hat{\boldsymbol{\pi}}\times\hat{\boldsymbol{\pi}} = \frac{iq\hbar}{c}\boldsymbol{B}.$$
$$[v_i, v_j] = \frac{iq\hbar}{m^2c}\epsilon_{ijk}B_k.$$
$$[\hat{\boldsymbol{v}},\hat{\boldsymbol{v}}^2] = \frac{iq\hbar}{m^2c}(\boldsymbol{v}\times\boldsymbol{B} - \boldsymbol{B}\times\boldsymbol{v}) \leftrightarrow [v_i,\boldsymbol{v^2}] = \frac{iq\hbar}{m^2c}\epsilon_{ijk}(\hat{v}_j B_k - B_j\hat{v}_k).$$

2. Rederive Newton-Lorentz's quation.
3. Order of magnitude analysis:

$$(1)\ \frac{q^2}{c^2}\boldsymbol{A}^2 \text{ vs. } \frac{q}{c}\boldsymbol{A}\cdot\hat{\boldsymbol{p}};\quad (2)\ \hat{H}_E \text{ vs. } \hat{H}_M.$$

4. Verify that $\boldsymbol{A} = \dfrac{1}{2}\boldsymbol{B}\times\boldsymbol{x}$ is correct, and give the condition that satisfies this result.
5. Rederive the Lagrangian and Hamiltonian for particles in EM field.
6. Compare the kinetic and canonical momentum for particles in EM field.

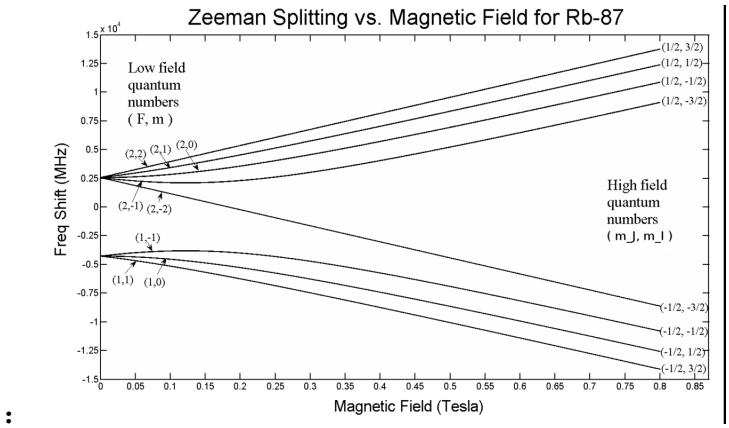
Lecture Notes 24 Zeeman Effect

Contents

- Basics;
- Theoretical Analysis of Normal Zeeman Effect;
- Theoretical Analysisi of Anormalous Zeeman Effect;
- Summary.

1. Basics:

The Zeeman effect is the effect of splitting of a spectral line into several components in the presence of a static magnetic field. It is named after the Dutch physicist Pieter Zeeman, who discovered it in 1896 and thereby won a Nobel prize for this discovery. It is analogous to the Stark effect, the splitting of a spectral line into several components in the presence of an electric field. Also similar to the Stark effect, transitions between different components have, in general, different intensities, with some being entirely forbidden (in the dipole approximation), as governed by the selection rules.



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Fig. 24: Experiment of Zeeman effect.

2. Theoretical Analysis of Normal Zeeman Effect

Non-relativistic quantum mechanics gives the interaction Hamiltonian for charged particles in the EM field as:

$$\hat{H}_{\rm M} = -\hat{\boldsymbol{\mu}}_L \cdot \boldsymbol{B} = \mu_{\rm B} B(\hat{L}_z/\hbar).$$

phenomena	magnetic field	theory	spectral line
Normal Zeeman	strong	CM/QM (NR)	uniform
Anormalous Zeeman	weak	QM (R)	non-uniform
Paschen-Back	strong	QM (R)	uniform

表 1: Different Zeeman effect.

Take the direction of the magnetic field as the quantum axis ($z-$axis), one can have the free Hamiltonian of the charged particles:

$$\hat{H}^{(0)} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{e^2}{r} \to |nlm_l\rangle.$$

We know that $(\hat{H}^{(0)}, \hat{\boldsymbol{L}}^2, \hat{L}_z)$ have the simultaneous eigenstates and they form a CSCO. So we can use three good quantum number n, l, m_l, to describe the state of the system. Also, we find that $|nlm_l\rangle$ is also the eigenstate of $\hat{H}_{\rm M}$:

$$\langle nlm_l|\hat{H}_{\rm M}|nlm_l\rangle = \Big(\frac{\mu_{\rm B}B}{\hbar}\Big)\langle nlm_l|\hat{L}_z|nlm_l\rangle = m_l\mu_{\rm B}B.$$

Therefore, $|nlm_l\rangle$ is the eigenstate of the system's Hamiltonian, the corresponding energy eigenvalue is

$$E_{nlm_l} = E_n^{(0)} + \mu_{\rm B}Bm_l.$$

We do some magnitude analyses here, for further discussions.

$$\hat{H}^{(0)} = E_n^{(0)} = \frac{1}{2n^2}(\alpha^2 mc^2), \quad \alpha = \frac{e^2}{\hbar c} = \frac{1}{137} = \frac{\lambda\!\!\!^{-}}{a_0},$$

where α is the fine structure constant, $\lambda\!\!\!^{-}$ is the reduced Compton wavelength. Normally, we have $\hat{H}_{\rm M} \ll \hat{H}^{(0)}$.

3. Theoretical Analysis of Anormalous Zeeman Effect

In relativistic theory, we need to take the spin into consideration. Review some properties of the Hydrogen atom:

a) Eigenstates and CSCO:

$$|nlm_l sm_s\rangle = |nlm_l\rangle \otimes |sm_s\rangle = |nlm_l m_s\rangle.$$

The CSCO and the corresponding good quantum numbers are:

$$\begin{aligned} &\text{CSCO:} && (\hat{H}^{(0)}, \hat{\boldsymbol{L}}^2, \hat{L}_z, \hat{\boldsymbol{s}}^2, \hat{s}_z), \\ &\text{good quantum numbers:} && (n, l, m_l, s, m_s). \end{aligned}$$

b) Some important constant in magnitude analyses:

Fine structure constant/Sommerfield constant: $\alpha = 1/137$,
Bohr radius: $a_0 = 0.52 \times 10^{-10}\text{m}$,
Bohr magneton: $\mu_{\text{B}} = e\hbar/2mc$.

$$\left|\frac{\mu_{\text{B}} B}{e a_0 \epsilon}\right| \sim \frac{\mu_{\text{B}}}{e a_0} = \frac{e\hbar}{2mc} \cdot \frac{1}{e a_0} \sim \left(\frac{\hbar}{mc}\right)/a_0 \to \left|\frac{\delta H_{\text{M}}}{\delta H_E}\right| \sim \alpha.$$

c) Fine sturcture analyses:

The free Hamiltonian writes:

$$\hat{H}^{(0)} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{e^2}{r} + \underline{a_r \hat{\boldsymbol{p}}^4} + \underline{a_{LS} \xi(r) \boldsymbol{S} \cdot \boldsymbol{L}} + \underline{\delta \hat{H}_{\text{Darwin}}}$$

The first term is the correction of kinetic energy in relativistic theory, the second term is due to the spin-orbital coupling, and the third term is the Darwin term, which takes non-zero value only when $l = 0$.

Consider the commutation relations:

$$[\hat{L}_i, V(r)] = 0, \quad [\hat{L}_i, \xi(r)] = 0,$$

while

$$\begin{cases} [\hat{L}_i, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}] = [\hat{L}_i, \hat{L}_j]\hat{S}_j = i\hbar\epsilon_{ijk}\hat{L}_k\hat{S}_j \neq 0, \\ [\hat{S}_i, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}] = \hat{L}_j[\hat{S}_i, \hat{S}_j] = i\hbar\epsilon_{ijk}\hat{L}_j\hat{S}_k \neq 0. \end{cases}$$

So, $(\hat{L}_z, \hat{S}_z)$ do not commute with the free Hamiltonian $\hat{H}^{(0)}$, and they cannot be included into the CSCO. Also, we have:

$$\begin{cases} [\hat{\boldsymbol{L}}^2, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}] = [\hat{\boldsymbol{L}}^2, \hat{L}_j]\hat{S}_j = 0, \\ [\hat{\boldsymbol{S}}^2, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}] = \hat{L}_j[\hat{\boldsymbol{S}}^2, \hat{S}_j] = 0. \end{cases}$$

So $(\hat{\boldsymbol{L}}^2, \hat{\boldsymbol{S}}^2)$ can be added into the CSCO. Define the total angular momentum (of the

electron) $\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$, and note that:

$$\begin{aligned}&[\hat{J}_i, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}] = [\hat{L}_i, \hat{L}_j]\hat{S}_j + \hat{L}_j[\hat{S}_i, \hat{S}_j] \\ =&i\hbar\epsilon_{ijk}(\hat{L}_k\hat{S}_j + \hat{L}_j\hat{S}_k) \equiv 0\end{aligned}$$

$$[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}] = [\hat{\boldsymbol{L}}^2 + \hat{\boldsymbol{L}}^2 + 2\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}, \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}] = 0$$

So the CSCO is $(\hat{H}^{(0)}, \hat{\boldsymbol{L}}^2, \hat{\boldsymbol{S}}^2, \hat{\boldsymbol{J}}^2, \hat{J}_z)$, the corresponding good quantum numbers are (n, l, s, j, m_j). The simultaneous eigenstates are $|nlsjm_j\rangle$.

$$\begin{aligned}|jm\rangle =& \sum_{m_1+m_2=m} |j_1m_1j_2m_2\rangle\underline{\langle j_1m_1j_2m_2|jm\rangle} \\ =& \sum_{m_l+m_s=m} |lm_lsm_s\rangle\underline{\langle lm_lsm_s|jm\rangle} \qquad (m=-j,\cdots,j; \quad j=|l-s|,\cdots,l+s).\end{aligned}$$

Now let's consider the interaction Hamiltonian. Since

$$\hat{H}_{\mathrm{M}} = -(\hat{\boldsymbol{\mu}}_L + \hat{\boldsymbol{\mu}}_S) \cdot \boldsymbol{B} = \mu_{\mathrm{B}}B(\hat{L}_z + 2\hat{S}_z)/\hbar,$$

one has

$$\begin{aligned}&\langle nljm_j|\hat{H}_{\mathrm{M}}|nljm_j\rangle \\ =&\frac{\mu_{\mathrm{B}}B}{\hbar}\left[\langle nljm_j|(\hat{L}_z + \hat{S}_z)|nljm_j\rangle + \langle nljm_j|\hat{S}_z|nljm_j\rangle\right] \\ =&\frac{\mu_{\mathrm{B}}B}{\hbar}\left[\langle nljm_j|\hat{J}_z|nljm_j\rangle + \langle nljm_j|\hat{S}_z|nljm_j\rangle\right] \\ =&m_j\mu_{\mathrm{B}}B + \frac{\mu_{\mathrm{B}}B}{\hbar}\langle nljm_j|\hat{S}_z|nljm_j\rangle\end{aligned}$$

To calculate $\langle nljm_j|\hat{S}_z|nljm_j\rangle$, we will first introduce *Projection Theorem* (投影定理):

$$\boxed{\langle jm|\hat{\boldsymbol{V}}|jm\rangle = \frac{\langle jm|(\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}})\hat{\boldsymbol{J}}|jm\rangle}{\langle jm|\hat{\boldsymbol{J}}^2|jm\rangle} = \frac{\langle jm|(\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}})\hat{\boldsymbol{J}}|jm\rangle}{\hbar^2 j(j+1)}.}$$

So one has (let $\hat{\boldsymbol{V}} = \hat{\boldsymbol{S}}$):

$$\langle jm_j|\hat{S}_z|jm_j\rangle = \frac{\langle jm_j|(\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{J}})\hat{J}_z|jm_j\rangle}{\langle jm_j|\hat{\boldsymbol{J}}^2|jm_j\rangle} = \frac{\hbar m_j\langle jm_j|(\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{J}})|jm_j\rangle}{\hbar^2 j(j+1)},$$

and

$$[\hat{J}_i, \hat{S}_i] = i\hbar\epsilon_{iik}\hat{S}_k \equiv 0 \to \hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{J}} = \hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{S}}.$$

So one has

$$\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{J}}=\frac{1}{2}[\hat{\boldsymbol{S}}^2+\hat{\boldsymbol{J}}^2-(\hat{\boldsymbol{J}}-\hat{\boldsymbol{S}})^2]=\frac{1}{2}(\hat{\boldsymbol{S}}^2+\hat{\boldsymbol{J}}^2-\hat{\boldsymbol{L}}^2).$$

Therefore

$$\langle jm|(\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{J}})|jm\rangle=\frac{1}{2}\langle jm|[\hat{\boldsymbol{S}}^2+\hat{\boldsymbol{J}}^2-(\hat{\boldsymbol{J}}-\hat{\boldsymbol{S}})^2]|jm\rangle=\frac{\hbar^2}{2}[j(j+1)+s(s+1)-l(l+1)].$$

Thus, we have

$$\langle jm_j|\hat{S}_z|jm_j\rangle=\frac{\hbar m_j}{\hbar^2 j(j+1)}\cdot\frac{\hbar^2}{2}[j(j+1)+\frac{3}{4}-l(l+1)]=\hbar m_j\frac{j(j+1)+\frac{3}{4}-l(l+1)}{2j(j+1)}.$$

$$\Delta E=\langle jm_j|\hat{H}_{\mathrm{M}}|jm_j\rangle=m_j\big[1+\frac{j(j+1)+\frac{3}{4}-l(l+1)}{2j(j+1)}\big]\cdot\mu_{\mathrm{B}}B=m_j g_j\mu_{\mathrm{B}}B.$$

The interaction energy is

$$\Delta E=m_j g_j\mu_{\mathrm{B}}B,$$

where g_j is the Landé factor

$$\boxed{g_j=1+\frac{j(j+1)+\frac{3}{4}-l(l+1)}{2j(j+1)}.}$$

In the above case, $\mu_{\mathrm{B}}\boldsymbol{B}\ll\xi(r)\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{L}}\sim\alpha^4mc^2$, the system is put under a weak field.

When the field is strong, that is $\mu_{\mathrm{B}}B\in[\alpha^2(mc^2),\alpha^4(mc^2)]$, the fine structrue can be ignored, so one has:

$$\hat{H}=\frac{\hat{\boldsymbol{p}}^2}{2m}-\frac{e^2}{r}+\mu_{\mathrm{B}}B(L_z+2S_z)/\hbar.$$

The energy shift is:

$$\Delta E=\langle nlm_lm_s|\hat{H}_{\mathrm{M}}|nlm_lm_s\rangle=\mu_{\mathrm{B}}B(m_l+2m_s).\quad\begin{cases}m_l=-l,\cdots,l;\\ m_s=-\dfrac{1}{2},\cdots,\dfrac{1}{2}.\end{cases}$$

Substitude $m_s=\pm\dfrac{1}{2}$ into the expression, and one yields:

$$\Delta E=\mu_{\mathrm{B}}B(m_l\pm1).$$

The shift of energy levels is uniform, but there are overlaps in the energy level.

Finally, we give the proof of the projection theorem.

(1) $[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{V}}] = 2i\hbar[\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}} - i\hbar\hat{\boldsymbol{V}}]$

$$\begin{aligned}
[\hat{J}_i \cdot \hat{J}_i, \hat{V}_j] &= [\hat{J}_i, \hat{V}_j]\hat{J}_i + \hat{J}_i[\hat{J}_i, \hat{V}_j] \\
&= i\hbar\epsilon_{ijk}(\hat{V}_k\hat{J}_i + \hat{J}_i\hat{V}_k) \\
&= i\hbar\epsilon_{ijk}(2\hat{V}_k\hat{J}_i + i\hbar\epsilon_{ikl}\hat{V}_l) \\
&= 2i\hbar(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}})_j - \hbar^2\epsilon_{ijk}\epsilon_{kli}V_l \\
&= 2i\hbar(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}})_j - \hbar^2(\delta_{il}\delta_{ji} - \delta_{ii}\delta_{jl})\hat{V}_l \\
&= 2i\hbar(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}})_j + 2\hbar^2\hat{V}_j. \\
\Longrightarrow [\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{V}}] &= 2i\hbar(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}) + 2\hbar^2\hat{\boldsymbol{V}} = 2i\hbar[\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}} - i\hbar\hat{\boldsymbol{V}}].
\end{aligned}$$

(2) $\dfrac{1}{(2i\hbar)^2}\Big[\hat{\boldsymbol{J}}^2, [\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{V}}]\Big] = (\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}})\hat{\boldsymbol{J}} - \dfrac{1}{2}(\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}}^2 + \hat{\boldsymbol{J}}^2 \cdot \hat{\boldsymbol{V}})$

$$\begin{aligned}
\Big[\hat{\boldsymbol{J}}^2, [\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{V}}]\Big] &= 2i\hbar[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{V}}] \times \hat{\boldsymbol{J}} + 2\hbar^2[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{V}}] \\
&= 2i\hbar(2i\hbar\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}} + 2\hbar^2\hat{\boldsymbol{V}}) \times \hat{\boldsymbol{J}} + 2\hbar^2[2i\hbar\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}} + 2\hbar^2\hat{\boldsymbol{V}}] \\
&= -4\hbar^2(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}) \times \hat{\boldsymbol{J}} + 4i\hbar^3(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}) + 4i\hbar^3(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}) + 4\hbar^4\hat{\boldsymbol{V}} \\
&= (2i\hbar)^2\big[(\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}})\hat{\boldsymbol{J}} - \hat{\boldsymbol{V}}\hat{\boldsymbol{J}}^2 + i\hbar(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}) - 2i\hbar(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}) - \hbar^2\hat{\boldsymbol{V}}\big] \\
&= (2i\hbar)^2\big[(\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}})\hat{\boldsymbol{J}} - \hat{\boldsymbol{V}}\hat{\boldsymbol{J}}^2 + i\hbar(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}) - \frac{1}{2}[\hat{\boldsymbol{J}}^2\hat{\boldsymbol{V}} - \hat{\boldsymbol{V}}\hat{\boldsymbol{J}}^2] - i\hbar\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}\big] \\
&= (2i\hbar)^2\big[(\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}})\hat{\boldsymbol{J}} - \frac{1}{2}(\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}}^2 + \hat{\boldsymbol{J}}^2 \cdot \hat{\boldsymbol{V}})\big].
\end{aligned}$$

Where we have used the relation:

$$(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}) \times \hat{\boldsymbol{J}} = (\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}})\hat{\boldsymbol{J}} - \hat{\boldsymbol{V}}\hat{\boldsymbol{J}}^2 + i\hbar(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}).$$

This can be proved easily:

$$\begin{aligned}
\Big[(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}}) \times \hat{\boldsymbol{J}}\Big]_i &= \epsilon_{ijk}\epsilon_{jlm}\hat{V}_l\hat{J}_m\hat{J}_k \\
&= (\delta_{kl}\delta_{im} - \delta_{km}\delta_{il})\hat{V}_l\hat{J}_m\hat{J}_k \\
&= \hat{V}_k\hat{J}_i\hat{J}_k - \hat{V}_i\hat{J}_k\hat{J}_k \\
&= \hat{V}_k[\hat{J}_k\hat{J}_i + i\hbar\epsilon_{ikj}\hat{J}_j] - (\hat{V}_i\hat{\boldsymbol{J}}^2) \\
&= \Big[(\hat{\boldsymbol{V}} \cdot \hat{\boldsymbol{J}})\hat{\boldsymbol{J}} - \hat{\boldsymbol{V}}\hat{\boldsymbol{J}}^2 + i\hbar(\hat{\boldsymbol{V}} \times \hat{\boldsymbol{J}})\Big]_i.
\end{aligned}$$

(3) Projection theorem:

$$\begin{aligned}&\langle jm|[\hat{\boldsymbol{J}}^2,[\hat{\boldsymbol{J}}^2,\hat{\boldsymbol{V}}]]|jm\rangle\\ =&j(j+1)\langle[\hat{\boldsymbol{J}}^2,\hat{\boldsymbol{V}}]\rangle - j(j+1)\langle[\hat{\boldsymbol{J}}^2,\hat{\boldsymbol{V}}]\rangle = 0.\end{aligned}$$

So,

$$\langle(\hat{\boldsymbol{V}}\cdot\hat{\boldsymbol{J}})\hat{\boldsymbol{J}}\rangle = \langle\hat{\boldsymbol{V}}\rangle j(j+1)\hbar^2.$$

4. Summary

"SOME IS SUPER":

S:	State postulate
O:	Observable postulate
M:	Measurement postulate
E:	Evolution postulate
IS:	Identical and Symmetrization postulate
S:	Scattering/Symmetry
U:	Unitary transfromation/Uncertainty principle
P:	Perturbation theory
E:	Electromagnetic field
R:	Rotation