Outlines of Quantum Physics

厄米算符 Hermitian Operator

1. 线性算符:
   $\hat{O}(c_1\Psi_1 + c_2\Psi_2) = c_1\hat{O}\Psi_1 + c_2\hat{O}\Psi_2$
   以下将只讨论线性算符
2. 波函数的内积
3. 算符的厄米共轭 $\hat{O}^+$
4. 厄米算符: $\hat{O}^+ = \hat{O}$

- Scalar Product
  $(\psi, \varphi) \equiv \int d\tau \psi^* \varphi$
- $(\psi, \psi) \geq 0$
  $(\psi, \varphi)^* = (\varphi, \psi)$
  $(\psi, \varphi_1 + \varphi_2) = (\psi, \varphi_1) + (\psi, \varphi_2)$
  $(\psi_1 + \psi_2, \varphi) = (\psi_1, \varphi) + (\psi_2, \varphi)$
  $(\psi, c\varphi) = c(\psi, \varphi)$
  $(c\psi, \varphi) = c^*(\psi, \varphi)$
- if $\forall \psi, \varphi$
  $(\psi, \hat{A}\varphi) = (\psi, \hat{B}\varphi)$,
  then $\hat{A} = \hat{B}$

厄米算符的基本性质

if $\hat{A}$, $\hat{B}$ are Hermitian, $\hat{A} \pm \hat{B}$ is Hermitian, but $\hat{A}\hat{B}$ NOT unless $\hat{A}\hat{B} = \hat{B}\hat{A}$

$\forall\Psi$, Hermitian 算符的平均值都是实数，逆命题也成立。 ⇒Proof

任何实验上可以观测的力学量，平均值都是实数，都是厄米算符

Eigenvalue and Eigenfunction of an Hermitian Operator

厄米算符的本征值必是实数

厄米算符属于不同本征值的本征函数正交——（正交性） ⇒Proof

力学量的本征函数系集可构成一个完备系，任何一个态函数都能用该函数系展开——（完备性）
可构成一个正交归一的完备函数集 (Complete Set)。

力学量的某个本征函数，只需要用属于相同本征值的那些本征函数展开——（子空间展开）

量子力学基本假设 Summary of Postulates in Q.M.

1. 用波函数描述微观体系的状态，是完全描述。(一般地，波函数单值、连续、平方可积，是 “品优函数”)
2. 任何可观测的物理量对应一个线性厄米算符，其本征函数可构成一个完备函数集。(此算符可由经典力学量作 $x \to \hat{x}$, $p_x \to -i\hbar\frac{\partial}{\partial x}$ 对应产生)
3. 关于可测力学量的任何可能的测量结果都是所对应算符 $\hat{F}$ 的一个本征值 f_m，测量后体系即 “坍缩” 到其相应的本征态 φ_m；
   每次测量得到 f_m 的概率：$|c_m|^2$，其中 $c_m = (\varphi_m, \Psi)$；
   测量平均值 $\langle F\rangle_\phi = \int \phi^* \hat{F}\phi\, d\tau$，其中 $\phi(q,t)$ 是一个已经归一的态函数。
   可构造 $\{\varphi_m\}$; $\quad \hat{F}\varphi_m = f_m\varphi_m$; $\quad (\varphi_m, \varphi_n) = \delta_{mn}$;
   $\forall\Psi$, $\Psi = \sum c_m\varphi_m$; $\quad (\varphi_m, \Psi) = c_m$; $\quad (\Psi, \Psi) = \sum_m |c_m|^2 = 1$
   $\langle F\rangle_\Psi = \bar{F} = (\Psi, \hat{F}\Psi) = \int \Psi^*\hat{F}\Psi\, d\tau = \sum_m f_m|c_m|^2$
4. 量子态的时间演化满足 Schrödinger 方程。

量子力学测量问题

问题：制备体系处于 Ψ 态，测量力学量 $\hat{F}$，量子力学有何预测?

- 解方程 $\hat{F}\phi_n = f_n\phi_n$，寻找 $\hat{F}$ 的本征值和本征函数;
- 构造 $\{\phi_n\}$，$(\phi_m, \phi_n) = \delta_{mn}$ 构成一个正交归一完备的函数集;
- 将 Ψ 在 $\{\phi_n\}$ 上展开，$\Psi = \sum_n c_n\phi_n$，展开系数 $c_n = (\phi_n, \Psi)$;
- 测得 f_n 的概率是 $|c_n|^2$，测量平均值是 $\sum_n f_n|c_n|^2$

"精确测量"的充分必要条件：被测态是该力学量的一个本征态

问题：如何求解方程 $\hat{F}\phi_n = f_n\phi_n$?

Dirac 符号

- 右矢（ket）$|\Psi\rangle$ 和左矢（bra ）$\langle\Phi|$
  - $|\Psi\rangle^{+} = \langle\Psi|$
- 标积 scalar product：$\langle\Phi|\Psi\rangle = \int d\tau \Phi^{*}\Psi$
- 正交完备集：$\{|k\rangle\}$,
  - 正交归一：$\langle k|j\rangle = \delta_{kj}$,
  - 完备性：$\sum_k |k\rangle\langle k| = 1$
- 态展开：$|\psi\rangle = \sum_k |k\rangle\langle k|\psi\rangle = \sum_k c_k|k\rangle$

对易式 Commutator

$$[A,B] \equiv AB - BA$$

$$[A,B] = -[B,A] \qquad [A,A] = 0 \qquad [A, const] = 0$$

$$[A, B+C] = [A,B] + [A,C]$$

$$[A, BC] = B[A,C] + [A,B]C$$

$$[AB, C] = A[B,C] + [A,C]B$$

$$[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$$

$$[A, B^n] = \sum_{s=0}^{n-1} B^s [A,B] B^{n-s-1}$$

例子，基本对易关系

$$[x, p_x] = i\hbar; \qquad [x, p_y] = 0; \qquad [x, y] = 0$$
$$[L_x, y] = i\hbar z; \qquad [L_x, z] = -i\hbar y; \qquad [L_x, x] = 0$$
$$[L_x, p_y] = i\hbar p_z; \qquad [L_x, p_z] = -i\hbar p_y; \qquad [L_x, p_x] = 0$$
$$[L_x, L_y] = i\hbar L_z; \qquad [L_x, L_z] = -i\hbar L_y;$$
$$[x_\alpha, p_\beta] = i\hbar\delta_{\alpha\beta}$$
$$[L_\alpha, x_\beta] = \sum_\gamma \epsilon_{\alpha\beta\gamma} i\hbar x_\gamma$$
$$[L_\alpha, p_\beta] = \sum_\gamma \epsilon_{\alpha\beta\gamma} i\hbar p_\gamma$$
$$[L_\alpha, L_\beta] = \sum_\gamma \epsilon_{\alpha\beta\gamma} i\hbar L_\gamma$$
$$[L^2, L_\alpha] = 0 \qquad L_\pm = L_x \pm iL_y \qquad [L_z, L_\pm] = \pm\hbar L_\pm$$

对易子与测不准关系

$\hat{A}$, $\hat{B}$ are Hermitian, $\Longrightarrow \forall\Psi$, $\sqrt{\overline{(\Delta A)^2} \cdot \overline{(\Delta B)^2}} \geq \frac{1}{2}|\overline{[A, B]}|$

⇒Proof

一般地，若 $\hat{A}$、$\hat{B}$ 不对易，
则不同时精确可测量（有确定的测量值），不能有共同的本征态。

$$\forall\Psi, \qquad \delta x \delta p \geq \hbar/2$$

但不排除恰好某个态上 $\overline{[A, B]}|_{\psi} = 0$，
使得即使 $\hat{A}$、$\hat{B}$ 不对易，
也可能存在个别的态，使得 $\hat{A}$、$\hat{B}$ 可同时精确测量（共同本征态）。

共同本征态

若 $[\hat{A}, \hat{B}] = 0$，
则**存在**完备函数集 $\{\varphi_i\}$，
φ_i 是 A，B 的共同本征态；
反之亦成立。

一般选取一组**两两对易**的力学量
共同本征函数集作为基函数集，(构成表象)，
任何波函数均可以在此基函数集上展开。

if $[\hat{A}, \hat{B}] = 0, \quad \hat{A}|i\rangle = a_i|i\rangle, \quad \hat{A}|j\rangle = a_j|j\rangle, \quad a_i \neq a_j$
then $\langle i|\hat{B}|j\rangle = 0$

谐振子的代数解法，a, a^+ 算符

$$H = \frac{1}{2}(x^2 + p^2), \qquad [x, p] = i$$

$$a = \frac{1}{\sqrt{2}}(x + ip), \qquad a^+ = \frac{1}{\sqrt{2}}(x - ip)$$

$$[a, a^+] = 1, \qquad N = a^+ a$$

$$N|n\rangle = n|n\rangle, \qquad H|n\rangle = (n + 1/2)|n\rangle$$

$$a^+|n\rangle = \sqrt{n+1}|n+1\rangle, \qquad a|n\rangle = \sqrt{n}|n-1\rangle$$

⇒Proof

角动量的定义

定义

如果算符 $\hat{J}$ 满足:

$$
\begin{aligned}
[J_x, J_y] &= i\hbar J_z \\
[J_y, J_z] &= i\hbar J_x \\
[J_z, J_x] &= i\hbar J_y
\end{aligned}
$$

则称 $\hat{J}$ 是一个角动量算符

角动量的一般性质

角动量算符满足的基本对易关系：

$$
\begin{aligned}
[J_x, J_y] &= i\hbar J_z \\
[J_y, J_z] &= i\hbar J_x \\
[J_z, J_x] &= i\hbar J_y \\
[J^2, J_\alpha] &= 0
\end{aligned}
$$

$$
\begin{aligned}
J_\pm &= J_x \pm iJ_y \\
[J_z, J_\pm] &= \pm\hbar J_\pm \\
J_\pm J_\mp &= J^2 - J_z^2 \pm \hbar J_z \\
J_+J_- - J_-J_+ &= 2\hbar J_z \\
J_+J_- + J_-J_+ &= 2(J^2 - J_z^2)
\end{aligned}
$$

仅由这些对易关系可证明： 证明

$$
\begin{aligned}
J^2|jm\rangle &= j(j+1)\hbar^2|jm\rangle \\
J_z|jm\rangle &= m\hbar|jm\rangle \\
J_\pm|jm\rangle &= \hbar\sqrt{(j\mp m)(j\pm m+1)}|jm\pm 1\rangle
\end{aligned}
$$

$$
j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \cdots \qquad m = -j, -j+1, \cdots j-1, j
$$

表象 Representation

选定一个（组）力学量 $\hat{G}$，其本征函数集 $\{|k\rangle\}$，构造成正交归一的完备基矢，体系的任一态 $|\psi\rangle$ 即可以在其下展开，此即为 $\hat{G}$ 表象。
显然，选择不同的 $\hat{G}$，就选择了不同的表象。

波函数在 $\{|k\rangle\}$ 表象中的表示（态矢）

$$
\begin{aligned}
|\psi\rangle &= \sum_k |k\rangle\langle k|\psi\rangle \\
&= \sum_k c_k|k\rangle \\
c_k &= \langle k|\psi\rangle
\end{aligned}
$$

即在**该表象下**，
一个波函数与一个列向量
$(c_1, c_2, \cdots, c_n, \cdots)$
相互对应。

力学量算符的矩阵表示

力学量 $\hat{F}$, 作用于量子态 $|\psi\rangle$，在由 $\hat{G}$ 本征函数集 $\{|k\rangle\}$ 构成的表象下，

$$
\begin{aligned}
\hat{F}|\psi\rangle &= |\phi\rangle \\
|\psi\rangle &= \sum_k a_k|k\rangle \\
|\phi\rangle &= \sum_k b_k|k\rangle
\end{aligned}
$$

$$
\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \overset{F}{\Rightarrow} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix}
$$

$\sum_k b_k|k\rangle = \hat{F}\sum_k a_k|k\rangle = \sum_k a_k\hat{F}|k\rangle$
$\Rightarrow \forall m,$
$\langle m|\sum_k b_k|k\rangle = \langle m|\sum_k a_k\hat{F}|k\rangle$
$\because \langle m|k\rangle = \delta_{mk}$
$\therefore b_m = \sum a_k\langle m|\hat{F}|k\rangle = \sum_k F_{mk}a_k$

$$
\begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} & & \\ & F_{mk} & \\ & & \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}
$$

力学量算符的矩阵表示

- 很明显，矩阵 $\{F_{mn}\}$ 与 $|\psi\rangle$、$|\phi\rangle$ 都无关，
  它刻画了力学量 $\hat{F}$ **在** $\{|k\rangle\}$ **表象（由** $\hat{G}$ **确定的！）下**的性质，
  即是该力学量在该表象中的矩阵表示。
- 注意，构成表象的力学量 $\hat{G}$ 自身在该表象中的矩阵表示应是已经对角化的，每个对角矩阵元即是对应的本征值。
- 在该表象中力学量 $\hat{F}$ 的本征值（向量）问题，
  即为该矩阵 $\{F_{mn}\}$ 的特征值（向量）问题。
  即求解矩阵 P: $P^{-1}FP = diag\{\ell_1, \cdots, \ell_n, \cdots\}$
  求得的 ℓ_n 是本征值，矩阵 P 就是由对应的特征列向量组成的矩阵；每一个特征向量所对应的波函数即是相应本征值对应的一个本征态。

角动量算符的矩阵元

利用 $J_{\pm}|jm\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}|jm \pm 1\rangle$
及 $J_x = \frac{1}{2}(J_+ + J_-)$、$J_y = \frac{1}{2i}(J_+ - J_-)$
写出 $\{|j\,m\rangle\}$ 基矢系下 J_x 和 J_y 的矩阵形式;
矩阵中只有哪些矩阵元是非零的?

$j = 1/2$，定义 Pauli 矩阵:

$$J_\alpha = \frac{\hbar}{2}\sigma_\alpha; \quad \alpha = x, y, z$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Puzzle：作为 “矢量” 的角动量。

求解量子力学测量问题

问题：制备体系处于 $|\Psi\rangle$ 态，测量力学量 $\hat{F}$，量子力学有何预测?

1. 选择合适的表象：力学量算符 $\hat{G}$ 的正交归一完备本征态集 $\{|k\rangle\}$;
2. 在该表象下写出待讨论力学量算符 $\hat{F}$ 和波函数 $|\Psi\rangle$ 的表示;
   $F_{mn} = \langle m|F|n\rangle$； $|\Psi\rangle = \sum_k a_k|k\rangle$
3. F 矩阵对角化，$P^{-1}FP = diag\{\ell_1, \cdots, \ell_n, \cdots\}$，即得到 $\hat{F}$ 的本征值 ℓ_i 和相应的（$\hat{G}$ 表象下的）本征态 $|\phi_i\rangle = \sum_k P_{ik}|k\rangle$;
4. 将 $|\Psi\rangle$ 在 $\hat{F}$ 的各个本征态上投影，$|\Psi\rangle = \sum_i c_i|\phi_i\rangle$;
   $c_i = \langle\phi_i|\Psi\rangle = \sum_k P_{ik}a_k$;
5. 测得 ℓ_i 的概率是 $|c_i|^2$，测量平均值是 $\sum_i \ell_i|c_i|^2$

Magnetic Moment of a Circulating Flow of Charge

$$\begin{aligned}\vec{\mu}_\ell &= I\vec{A} \\ I &= -e/T = -e\omega/2\pi \\ \vec{\mu}_\ell &= -e\vec{r}\times\vec{v}/2 \\ &= -\frac{e}{2m_e}\vec{L} \\ &= -\mu_B\vec{L}/\hbar \\ \mu_{\ell z} &= -m_\ell\mu_B\end{aligned}$$

玻尔磁子Bohr magneton

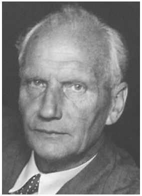
$\mu_B = \frac{e\hbar}{2m_e} = 9.274\,010\,078\,3(28)\times 10^{-24}(\mathrm{J\cdot T^{-1}}) \approx 58\mu\mathrm{eV/T}$

Magnet in a B field:

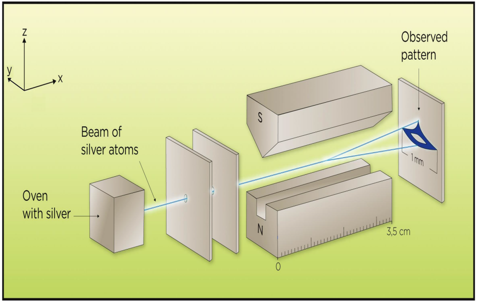
Torque: $\vec{\tau} = \vec{\mu}\times\vec{B}$

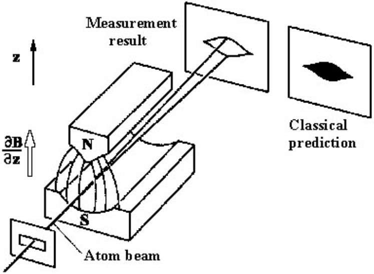
Potential energy: $U = -\vec{\mu}\cdot\vec{B} = -B\mu_z$

Stern-Gerlach experiment



1922, Otto Stern$_{NP1943}$ (1888-1969) & Walther Gerlach (1889-1979), University of Frankfurt





$$\vec{F} = -\nabla U = -\nabla(-\vec{\mu} \cdot \vec{B}), \qquad F_z = \mu_z \frac{\partial B_z}{\partial z}$$

Electron Spin

Hypothesis of Electron Spin

- 1922, Otto Stern & Walther Gerlach, University of Frankfurt
- 1925, Uhlenbeck and Goudsmit: explaining the Zeeman effect. Kronig discarded, objection from Pauli, Krammers and Heisenberg
- 1928 P.A.M.Dirac: Electron has a spin in relativistic Quantum Mechanics.
- Spin has no classical analog! 自旋没有经典对应

Magnetic moment of electron spin

$\vec{\mu}_s = -g_s \mu_B \vec{s}/\hbar, \qquad \mu_{sz} = -g_s m_s \mu_B, \qquad \mu_B = \frac{e\hbar}{2m_e}$

$g_s \approx 2.0023...$ (Note. $g_\ell = 1$)

Quantum Electrodynamics (QED): $g_s = 2[1 + \frac{\alpha}{2\pi} + O(\alpha^2)]$,

$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c}, \qquad 1/\alpha = 137.035\,999\,084(21)$

Exchange of Identical Particles

Identical Particles: must be indistinguishable!

Non-classical, Absolutely Quantum!

置换算符 Permutation/exchange Operator P_{ij}

$$\begin{aligned}
\mathbf{P}_{ij}\Psi(q_1,\cdots q_i,\cdots q_j,\cdots q_N) &= \Psi(q_1,\cdots q_j,\cdots q_i,\cdots q_N) \\
&= \lambda\Psi(q_1,\cdots q_i,\cdots q_j,\cdots q_N) \\
\mathbf{P}_{ij}^2\Psi = \Psi, &\qquad \lambda^2 = 1,\ \ \lambda = \pm 1
\end{aligned}$$

Symmetric: Bosons; Anti-symmetric: Fermions.
Symmetrization Postulate: 任何微观粒子必是二者之一（无混和）

Fermion and Boson

Fundamental Particles

- $\lambda = 1$, Boson: π (pion) ($s = 0$), photon ($s = 1$) ...
  Integral spin, Bose-Einstein distribution.
- $\lambda = -1$, Fermion: electron, proton, neutron ($s = 1/2$) ...
  Half-integral spin, Fermi-Dirac distribution.

Identical Composite Particles, **without considering any change in the internal structures:** number of Fermions consisted in the "particle":

- odd: Fermion, ^{3}He nucleus ...
- even: Boson, ^{4}He, D(^{2}H)...

Wavefunction of a system consisted of multiple identical particles:

- Exchange of two identical Bosons$P_{(B)ij}$, must be symmetric;
- Exchange of two identical Fermions $P_{(F)ij}$, must be anti-symmetric

Electronic wavefunction of Helium, ground state

Ground State of Helium

- spacial function: $1s(1)1s(2)$
  $\mathbf{P}_{12}[1s(1)1s(2)] = [1s(1)1s(2)]$, symmetric
- spin function: $\alpha(1)\alpha(2)$, $\alpha(1)\beta(2)$, $\beta(1)\alpha(2)$, $\beta(1)\beta(2)$
  Symmetric:
  - $\alpha(1)\alpha(2)$,
  - $\beta(1)\beta(2)$,
  - $[\alpha(1)\beta(2) + \beta(1)\alpha(2)]/\sqrt{2}$

  Anti-symmetric:
  - $[\alpha(1)\beta(2) - \beta(1)\alpha(2)]/\sqrt{2}$
- Physically correct Ψ must be anti-symmetric:
  $\psi(q_1, q_2) = [1s(1)1s(2)][\alpha(1)\beta(2) - \beta(1)\alpha(2)]/\sqrt{2}$

Electronic wavefunction of Helium, excited state

Excited States of Helium

- Spin function:
  Symmetric: $\alpha(1)\alpha(2)$, $\beta(1)\beta(2)$, $[\alpha(1)\beta(2)+\beta(1)\alpha(2)]/\sqrt{2}$
  Anti-symmetric: $[\alpha(1)\beta(2)-\beta(1)\alpha(2)]/\sqrt{2}$
- Spacial function: $1s(1)2s(2)$
  Symmetric: $[1s(1)2s(2)+2s(1)1s(2)]/\sqrt{2}$
  Anti-symmetric: $[1s(1)2s(2)-2s(1)1s(2)]/\sqrt{2}$
- Physically correct Ψ must be anti-symmetric:
  - $(1s2s)^3S_1$, spacial: anti-symmetric & spin: symmetric:
    $\psi(1,2)_1=[1s(1)2s(2)-2s(1)1s(2)]\alpha(1)\alpha(2)/\sqrt{2}$
    $\psi(1,2)_2=[1s(1)2s(2)-2s(1)1s(2)]\beta(1)\beta(2)/\sqrt{2}$
    $\psi(1,2)_3=[1s(1)2s(2)-2s(1)1s(2)][\alpha(1)\beta(2)+\beta(1)\alpha(2)]/2$
  - $(1s2s)^1S_0$, spacial: symmetric & spin: anti-symmetric:
    $\psi(1,2)_4=[1s(1)2s(2)+2s(1)1s(2)][\alpha(1)\beta(2)-\beta(1)\alpha(2)]/2$
    $E(^3S_1)<E(^1S_0)$

Ground State of Atomic Lithium, Pauli Exclusion Principle

Ground State of The Lithium Atom

- Spacial: could it be possible to have 3 electrons all in $1s$?
  $[1s(1)1s(2)1s(3)]$
  $\mathbf{P}_{ij}[1s(1)1s(2)1s(3)] = [1s(1)1s(2)1s(3)]$, symmetric
- Spin: $\alpha(1)\alpha(2)\alpha(3)$, $\alpha(1)\beta(2)\alpha(3)$, $\cdots$
  Make it symmetric or anti-symmetric for P_{12}, P_{13} & P_{23}
  Symmetric:
  1. $\alpha\alpha\alpha$
  2. $\beta\beta\beta$
  3. $[\alpha\alpha\beta + \alpha\beta\alpha + \beta\alpha\alpha]/\sqrt{3}$
  4. $[\alpha\beta\beta + \beta\beta\alpha + \beta\alpha\beta]/\sqrt{3}$

  Anti-symmetric: none
- Impossible to construct an anti-symmetric Ψ!

Wavefunction of a system consisted of identical particles

Total wavefuntion of N identical particles

$$\Phi = \phi_1(q_1)\phi_2(q_2)\cdots\phi_N(q_N)$$

Symmetric Wavefunctions of Bosons

$$\Phi^S = \frac{1}{\sqrt{N!}}\sum_{\mathbf{P}} \hat{\mathbf{P}}\phi_1(q_1)\phi_2(q_2)\cdots\phi_N(q_N)$$

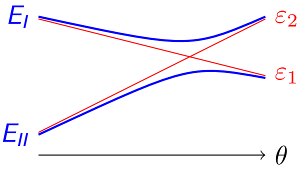
Anti-Symmetric Wavefunctions of Fermions, Slater Determinants

$$\Phi^A = \frac{1}{\sqrt{N!}}\sum_{\mathbf{P}}(-1)^P\hat{\mathbf{P}}\phi_1(q_1)\phi_2(q_2)\cdots\phi_N(q_N)$$
$$= \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(q_1) & \phi_1(q_2) & \cdots & \phi_1(q_N) \\ \phi_2(q_1) & \phi_2(q_2) & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \phi_N(q_1) & \phi_N(q_2) & \cdots & \phi_N(q_N) \end{vmatrix}$$

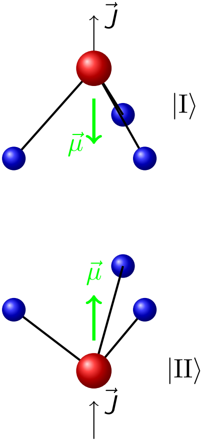
Two-State System

- Two state $|1\rangle$ and $|2\rangle$
- Hamiltonian:
  $$H = \begin{pmatrix} \varepsilon_1 & -h' \\ -h' & \varepsilon_2 \end{pmatrix}$$
  $$2\Delta = \varepsilon_1 - \varepsilon_2, \quad 2\varepsilon = (\varepsilon_1 + \varepsilon_2)$$
- $E_{I,II} = \varepsilon \pm \sqrt{\Delta^2 + h'^2}$
- If $\Delta \gg h'$:
  $$E \doteq \varepsilon \mp \Delta(1 + \frac{1}{2}\frac{h'^2}{\Delta^2})$$
  $$E_I \doteq \varepsilon_1 + \frac{h'^2}{2\Delta}$$
  $$E_{II} \doteq \varepsilon_2 - \frac{h'^2}{2\Delta}$$
- If $\Delta \ll h'$:
  $$E \doteq \varepsilon \pm h'(1 + \frac{1}{2}\frac{\Delta^2}{h'^2})$$
  $$E_I \doteq \varepsilon + h' + \frac{\Delta^2}{2h'}$$
  $$E_{II} \doteq \varepsilon - h' - \frac{\Delta^2}{2h'}$$

"Avoid Crossing"



Double States of the Ammonia Molecule*



- Base states: $|\mathrm{I}\rangle$ & $|\mathrm{II}\rangle$
- Hamiltonian: $\begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$
- Eigenvalues and eigenfunctions:
  $E_1 = E_0 - A$
  $E_2 = E_0 + A$
  $|1\rangle = \frac{1}{\sqrt{2}}(|\mathrm{I}\rangle - |\mathrm{II}\rangle)$
  $|2\rangle = \frac{1}{\sqrt{2}}(|\mathrm{I}\rangle + |\mathrm{II}\rangle)$
- $|\Psi\rangle = c_1|1\rangle + c_2|2\rangle = C_{\mathrm{I}}|\mathrm{I}\rangle + C_{\mathrm{II}}|\mathrm{II}\rangle$
  $\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} C_{\mathrm{I}} \\ C_{\mathrm{II}} \end{pmatrix}$

Double States of the Ammonia Molecule*

- Base states:

$|\Psi\rangle = c_1|1\rangle + c_2|2\rangle \qquad |\Psi\rangle = C_{\mathrm{I}}|\mathrm{I}\rangle + C_{\mathrm{II}}|\mathrm{II}\rangle$

- Hamiltonian:

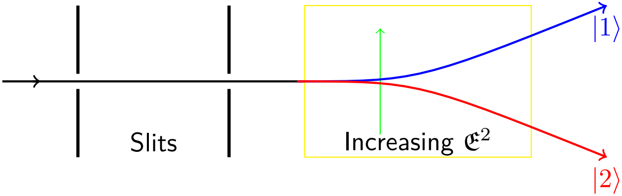
$$H = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \qquad H' = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$

- Evolution of states:
  if $|\Psi_{t=0}\rangle = a|1\rangle + b|2\rangle$, then $|\Psi_t\rangle = ae^{-iE_1t/\hbar}|1\rangle + be^{-iE_2t/\hbar}|2\rangle$
- if the system is in the state $|\mathrm{I}\rangle$ when $t = 0$:
  $|\Psi_{t=0}\rangle = |\mathrm{I}\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle$, $\quad |\Psi_t\rangle = C_{\mathrm{I}}(t)|\mathrm{I}\rangle + C_{\mathrm{II}}(t)|\mathrm{II}\rangle$
  $C_{\mathrm{I}}(t) = \frac{1}{2}e^{-iE_0t/\hbar}(e^{iAt/\hbar} + e^{-iAt/\hbar}) = e^{-iE_0t/\hbar}\cos(At/\hbar)$
  $C_{\mathrm{II}}(t) = ie^{-iE_0t/\hbar}\sin(At/\hbar)$
- $|C_{\mathrm{I}}(t)|^2 = \cos^2\frac{At}{\hbar} = (1+\cos\omega_0 t)/2$,
  $|C_{\mathrm{II}}(t)|^2 = \sin^2\frac{At}{\hbar} = (1-\cos\omega_0 t)/2$,
  $\omega_0 = 2A/\hbar$

Ammonia molecule in a static electric field*

If we apply a small electric field $\mathfrak{E}$:

- Hamiltonian (using bases $|\mathrm{I}\rangle$ & $|\mathrm{II}\rangle$):
  $$H_{\mathfrak{E}} = \begin{pmatrix} E_0 - \mu\mathfrak{E} & -A \\ -A & E_0 + \mu\mathfrak{E} \end{pmatrix}$$
- $E_1 = E_0 - \sqrt{A^2 + \mu^2\mathfrak{E}^2}, \quad E_2 = E_0 + \sqrt{A^2 + \mu^2\mathfrak{E}^2}$
- If the applied field is weak,
  $E_1 = E_0 - A - \frac{\mu^2\mathfrak{E}^2}{2A}, \quad E_2 = E_0 + A + \frac{\mu^2\mathfrak{E}^2}{2A}$
- Force on the molecule, Polarized beam:
  $F = \frac{\mu^2}{2A}\nabla\mathfrak{E}^2$

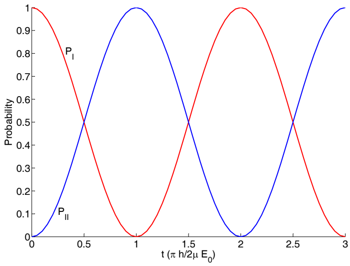


Rabi Oscillations

- Basis states: $|1\rangle$、$|2\rangle$, $|\Psi\rangle = c_1|1\rangle + c_2|2\rangle$,
  Time-dependent S.-Eq：
  $$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} E_1 & \mathcal{X}\mathfrak{E} \\ \mathcal{X}\mathfrak{E} & E_2 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$
- 令 $\omega_0 = (E_2 - E_1)/\hbar, \quad c_1 = \gamma_1(t)e^{-iE_1t/\hbar}, \quad c_2 = \gamma_2(t)e^{-iE_2t/\hbar}$
- $i\hbar\frac{d\gamma_1}{dt} = \mathcal{X}\mathfrak{E}(t)\gamma_2 e^{-i\omega_0 t}$
  $i\hbar\frac{d\gamma_2}{dt} = \mathcal{X}\mathfrak{E}(t)\gamma_1 e^{i\omega_0 t}$
- Periodically oscillating E-field: $\mathfrak{E} = \mathfrak{E}_0 \cos\omega t = \mathfrak{E}_0(e^{i\omega t} + e^{-i\omega t})/2$
  Rabi frequency is defined as: $\Omega = \mathcal{X}\mathfrak{E}_0/\hbar$
- $i\frac{d\gamma_1}{dt} = \frac{\Omega}{2}\gamma_2[e^{i(\omega+\omega_0)t} + e^{-i(\omega-\omega_0)t}]$
  $i\frac{d\gamma_2}{dt} = \frac{\Omega}{2}\gamma_1[e^{i(\omega-\omega_0)t} + e^{-i(\omega+\omega_0)t}]$

Rabi Frequency

- Ignoring the $e^{i(\omega+\omega_0)t}$ term; Let $\omega-\omega_0=\Delta$, then:
  $i\frac{d\gamma_1}{dt}=\frac{\Omega}{2}e^{-i\Delta t}\gamma_2, \qquad i\frac{d\gamma_2}{dt}=\frac{\Omega}{2}e^{i\Delta t}\gamma_1$
- If $\gamma_1|_{t=0}=1$, $\gamma_2|_{t=0}=0$, define $W=\sqrt{\Delta^2+\Omega^2}$, and we get,
  $|\gamma_1|^2+|\gamma_2|^2=1$
  $\gamma_1=e^{-i\Delta t/2}[\cos\frac{Wt}{2}+\frac{i\Delta}{W}\sin\frac{Wt}{2}]$
  $\gamma_2=-i\frac{\Omega}{W}e^{i\Delta t/2}\sin\frac{Wt}{2}$
- Possibility of system observed at $|2\rangle$ after time t:
  $P_2=\frac{\Omega^2}{W^2}\sin^2\frac{Wt}{2}=\frac{\Omega^2}{W^2}\frac{1-\cos Wt}{2}$
- $\Delta=0$: system oscillates between two states with Rabi frequency Ω:



If $\hat{F}$ is Hermitian, then $\forall\Psi$, $\bar{F} \in \mathbb{R}$

Hermitian 算符在任意一个态上的平均值都是实数

$\forall\Psi$

$$\begin{aligned} \bar{F} &= (\Psi, \hat{F}\Psi) \\ &= (\hat{F}\Psi, \Psi) \\ &= (\Psi, \hat{F}\Psi)^* \\ &= \bar{F}^* \end{aligned}$$

$\Longrightarrow$

$$\bar{F} \in \mathbb{R}$$

- $\hat{F}$ is Hermitian.
- $(\phi, \psi) = (\psi, \phi)^*$

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If $\forall\Psi$, $\bar{F}=\bar{F}^*$, then $\hat{F}$ is Hermitian.

如果一个算符在任意态上的平均值都是实数，这个算符是 Hermitian

- $\forall\psi$, $(\psi,\hat{F}\psi)=(\hat{F}\psi,\psi)$
- $(\phi_1+c\phi_2,\hat{F}\phi_1+c\hat{F}\phi_2)=$ $(\hat{F}\phi_1+c\hat{F}\phi_2,\phi_1+c\phi_2)$
- 左 $=(\phi_1,\hat{F}\phi_1)+|c|^2(\phi_2,\hat{F}\phi_2)+$ $c(\phi_1,\hat{F}\phi_2)+c^*(\phi_2,\hat{F}\phi_1)$
  右 $=(\hat{F}\phi_1,\phi_1)+|c|^2(\hat{F}\phi_2,\phi_2)+$ $c(\hat{F}\phi_1,\phi_2)+c^*(\hat{F}\phi_2,\phi_1)$
- $c[(\phi_1,\hat{F}\phi_2)-(\hat{F}\phi_1,\phi_2)]=$ $-c^*[(\phi_2,\hat{F}\phi_1)-(\hat{F}\phi_2,\phi_1)]$
- $(\phi_1,\hat{F}\phi_2)-(\hat{F}\phi_1,\phi_2)=$ $-(\phi_2,\hat{F}\phi_1)+(\hat{F}\phi_2,\phi_1)$
- $(\phi_1,\hat{F}\phi_2)-(\hat{F}\phi_1,\phi_2)=$ $(\phi_2,\hat{F}\phi_1)-(\hat{F}\phi_2,\phi_1)$
- $(\phi_1,\hat{F}\phi_2)-(\hat{F}\phi_1,\phi_2)=0$

- 即已知：$\forall\Psi$, $\bar{F}=\bar{F}^*$
  $\Leftrightarrow(\Psi,\hat{F}\Psi)=(\Psi,\hat{F}\Psi)^*$
  $=(\hat{F}\Psi,\Psi)$
  要证明：
  $\hat{F}$ Hermitian
  $\Leftrightarrow\forall\phi_1,\phi_2$,
  $(\phi_1,\hat{F}\phi_2)=(\hat{F}\phi_1,\phi_2)$
- 取 $\psi=\phi_1+c\phi_2$ 代入；
- $(\phi_1,\hat{F}\phi_1)=(\hat{F}\phi_1,\phi_1)$；
  $(\phi_2,\hat{F}\phi_2)=(\hat{F}\phi_2,\phi_2)$
- $\because c$ 任意，取 $c=1$,
- 取 $c=i$

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Eigenvalues and Eigenfunctions of Hermitian Operators

厄米算符的本征值是实数

$\hat{F}\phi_m = f_m\phi_m$, $\hat{F}$ is Hermitian,
$(\phi_m, \hat{F}\phi_m) = f_m \in \mathbb{R}$

厄米算符的属于不同本征值的本征函数正交

- $\hat{F}\phi_m = f_m\phi_m$
  $\hat{F}\phi_n = f_n\phi_n$
  $f_m \neq f_n$
- $(\phi_n, \hat{F}\phi_m) = (\hat{F}\phi_n, \phi_m)$

- $(\phi_n, \hat{F}\phi_m) = (\phi_n, f_m\phi_m) = f_m(\phi_n, \phi_m)$
- $(\hat{F}\phi_n, \phi_m) = (f_n\phi_n, \phi_m) = f_n^*(\phi_n, \phi_m) = f_n(\phi_n, \phi_m)$
- $(\phi_n, \phi_m)(f_m - f_n) = 0$
- $\because f_m \neq f_n$,
  $\therefore (\phi_n, \phi_m) = 0$

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Uncertainty Principle

测不准原理

if $\hat{A}$, $\hat{B}$ are Hermitian, then $\delta A \cdot \delta B \geq \frac{1}{2}|\overline{[\hat{A}, \hat{B}]}|$

Proof:

1. $[\hat{A}, \hat{B}] = i\hat{C}$,
   $\hat{C}^+ = \hat{C}$
2. $\forall\Psi$, $\sqrt{\overline{A^2} \cdot \overline{B^2}} \geq \frac{1}{2}|\overline{C}|$
3. $\Delta A = \hat{A} - \bar{A}$, $\Delta B = \hat{B} - \bar{B}$,
   $\sqrt{\overline{\Delta A^2} \cdot \overline{\Delta B^2}} \geq \frac{1}{2}|\overline{C}|$

$([\hat{A}, \hat{B}])^+$
$= (\hat{A}\hat{B} - \hat{B}\hat{A})^+$
$= \hat{B}^+\hat{A}^+ - \hat{A}^+\hat{B}^+$
$= \hat{B}\hat{A} - \hat{A}\hat{B}$
$= [\hat{B}, \hat{A}] = -[\hat{A}, \hat{B}]$
ΔA, ΔB are also Hermitian;
$[\Delta A, \Delta B] = [\hat{A}, \hat{B}]$
前面结论适用!

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$\forall\Psi,\ \sqrt{\overline{A^2}\cdot\overline{B^2}} \geq \frac{1}{2}|\overline{C}|$

$$I(\xi) = (\xi\hat{A}\Psi + i\hat{B}\Psi, \xi\hat{A}\Psi + i\hat{B}\Psi)$$
$$\forall\xi\in\mathbb{R},\ I(\xi)\geq 0$$

$$\begin{aligned} I(\xi) &= \xi^2(\hat{A}\Psi,\hat{A}\Psi) - i\xi(\hat{B}\Psi,\hat{A}\Psi) \\ &\quad + i\xi(\hat{A}\Psi,\hat{B}\Psi) + (\hat{B}\Psi,\hat{B}\Psi) \\ &= \xi^2(\Psi,\hat{A}^2\Psi) + i\xi(\Psi,\hat{A}\hat{B}\Psi) \\ &\quad - i\xi(\Psi,\hat{B}\hat{A}\Psi) + (\Psi,\hat{B}^2\Psi) \\ &= \xi^2\overline{A^2} - \xi\overline{C} + \overline{B^2} \end{aligned}$$

$$\overline{C}^2 \leq 4\overline{A^2}\cdot\overline{B^2}$$

- $\forall\psi,\ (\psi,\psi)\geq 0$
- $(c\phi,\psi) = c^*(\phi,\psi)$
- $\hat{F}$ is Hermitian $\Rightarrow$ $(\phi,\hat{F}\psi) = (\hat{F}\phi,\psi)$
- $\hat{A}^+ = \hat{A},\ \hat{B}^+ = \hat{B}$
- $[\hat{A},\hat{B}] = i\hat{C},\ \hat{C}^+ = \hat{C}$
- $\forall x\in\mathbb{R}$, $ax^2 + bx + c \geq 0$ $\Leftrightarrow b^2 \leq 4ac$

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谐振子的因式分解解法

Facterization method, Schrödinger, 1940

- $\hat{H} = \frac{1}{2}(\hat{x}^2 + \hat{p}^2)$
- $H = a^+ a + \frac{1}{2} = N + \frac{1}{2}$
  $[a, a^+] = 1$
- N 正定：$\forall \psi$, $\overline{N} \geq 0$
  设 $\{|\alpha\rangle\}$, $N|\alpha\rangle = \alpha|\alpha\rangle$
- 可证：
  $Na|\alpha\rangle = (\alpha - 1)a|\alpha\rangle$
  $Na^+|\alpha\rangle = (\alpha + 1)a^+|\alpha\rangle$
- 存在 $|0\rangle$, $N|0\rangle = 0$
- 则可以构造：
  $|1\rangle \sim a^+|0\rangle$, $|2\rangle \sim a^+|1\rangle \cdots$
  $|n\rangle = \frac{1}{\sqrt{n!}}(a^+)^n|0\rangle$
  $\langle n|n'\rangle = \delta_{n\,n'}$
  $N|n\rangle = n|n\rangle$

- 即 $a|\alpha\rangle$, $a^2|\alpha\rangle$, $\cdots$ 分别是 N 的本征值为 $\alpha - 1$, $\alpha - 2$, $\cdots$ 的本征函数；
- 而 N 正定，其本征值必不小于零；
- 必须存在一个最小的 α_0，使得：
  $a|\alpha_0\rangle = 0.$
- 而
  $N|\alpha_0\rangle = a^+ a|\alpha_0\rangle = 0|\alpha_0\rangle$
  即有 $\alpha_0 = 0$

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角动量本征值的代数解法 *
Eigenvalues of an Angular Momentum Operator

- $J^2|\lambda m\rangle = \lambda|\lambda m\rangle, \qquad J_z|\lambda m\rangle = m|\lambda m\rangle, \qquad (\hbar = 1)$
- If $\lambda' \neq \lambda$, $\langle\lambda' m'|J_\alpha|\lambda m\rangle = 0 \qquad \alpha = x, y, z, \pm$ proof
- $J_z(J_\pm|\lambda m\rangle) = (m \pm 1)(J_\pm|\lambda m\rangle)$, "Ladder Operators" proof
- $J^2 J_\pm^k|\lambda m\rangle = \lambda J_\pm^k|\lambda m\rangle, \qquad J_z^2 J_\pm^k|\lambda m\rangle = (m \pm k)^2 J_\pm^k|\lambda m\rangle$
  $\langle m \pm k|(J^2 - J_z^2)|m \pm k\rangle = (\lambda - (m \pm k)^2)\langle m \pm k|m \pm k\rangle$ proof
- $J^2 - J_z^2 = J_x^2 + J_y^2, \qquad \langle\psi|A^2|\psi\rangle \geq 0$ proof
- $\exists \overline{m}, \underline{m}, \qquad J_+|\overline{m}\rangle = 0, \qquad J_-|\underline{m}\rangle = 0$
- $\underline{m} = \overline{m} - n, \qquad \underline{m} = -\overline{m}$ proof
- $\overline{m} = j, \qquad \lambda = j(j+1), \qquad j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \cdots$

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角动量本征值的代数解法 *

If $\lambda' \neq \lambda$, $\langle \lambda' m' | J_\alpha | \lambda m \rangle = 0 \qquad \alpha = x, y, z, \pm$

$$\begin{aligned} \because \quad & [J^2, J_\alpha] = 0 \\ \therefore \quad & \langle \lambda' m' | J^2 J_\alpha - J_\alpha J^2 | \lambda m \rangle \\ = \quad & \lambda' \langle \lambda' m' | J_\alpha | \lambda m \rangle - \lambda \langle \lambda' m' | J_\alpha | \lambda m \rangle \\ = \quad & (\lambda' - \lambda) \langle \lambda' m' | J_\alpha | \lambda m \rangle \\ = \quad & 0. \end{aligned}$$

在 $\{|\lambda m\rangle\}$ 表象中，所有 J_α 的表示 (矩阵)，对 λ 都是 " 块" 对角化的。

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角动量本征值的代数解法 *

Ladder Operators

$J_z J_\pm |\lambda m\rangle = (m \pm 1) J_\pm |\lambda m\rangle$

$$
\begin{aligned}
\because \quad & [J_z, J_\pm] = \pm J_\pm \quad (\hbar = 1) \\
\therefore \quad & [J_z, J_\pm] |\lambda m\rangle = \pm J_\pm |\lambda m\rangle \\
\Rightarrow \quad & (J_z J_\pm - J_\pm J_z) |\lambda m\rangle = \pm J_\pm |\lambda m\rangle \\
\Rightarrow \quad & J_z J_\pm |\lambda m\rangle - m J_\pm |\lambda m\rangle = \pm J_\pm |\lambda m\rangle \\
\Rightarrow \quad & J_z (J_\pm |\lambda m\rangle) = (m \pm 1)(J_\pm |\lambda m\rangle).
\end{aligned}
$$

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角动量本征值的代数解法 *

$$\langle m \pm k|(J^2 - J_z^2)|m \pm k\rangle = (\lambda - (m \pm k)^2)\langle m \pm k|m \pm k\rangle$$

$$\begin{aligned} [J^2, J_\pm] = 0 \quad &\Rightarrow \quad J^2 J_\pm^k = J_\pm^k J^2 \\ &\Rightarrow \quad J^2 J_\pm^k|\lambda m\rangle = \lambda J_\pm^k|\lambda m\rangle \\ J_z J_\pm|\lambda m\rangle = (m \pm 1)J_\pm|\lambda m\rangle \quad &\Rightarrow \quad J_z J_\pm^k|\lambda m\rangle = (m \pm k)J_\pm^k|\lambda m\rangle \end{aligned}$$

固定 λ，记 $J_\pm^k|\lambda m\rangle \equiv |m \pm k\rangle$， $k \in \mathbb{Z}$

$$\begin{aligned} J^2|m \pm k\rangle &= \lambda|m \pm k\rangle \\ J_z|m \pm k\rangle &= (m \pm k)|m \pm k\rangle \\ J_z^2|m \pm k\rangle &= (m \pm k)^2|m \pm k\rangle \\ (J^2 - J_z^2)|m \pm k\rangle &= \{\lambda - (m \pm k)^2\}|m \pm k\rangle. \end{aligned}$$

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角动量本征值的代数解法 *

If A is Hermitian, $\forall\psi$, $\overline{A^2} \geq 0$

$$\begin{aligned} \overline{A^2} &= (\psi, A^2\psi) \\ &= (A\psi, A\psi) \\ &\geq 0. \end{aligned}$$

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角动量本征值的代数解法 *

$\underline{m} = -\overline{m}$

$J_\pm J_\mp = J^2 - J_z^2 \pm J_z$

$$
\begin{aligned}
& J_-|\underline{m}\rangle = 0 \\
& J_+J_-|\underline{m}\rangle = (\lambda - \underline{m}^2 + \underline{m})|\underline{m}\rangle = 0 \\
\Rightarrow \quad & \lambda = \underline{m}^2 - \underline{m} \\
& J_+|\overline{m}\rangle = 0 \\
& J_-J_+|\overline{m}\rangle = (\lambda - \overline{m}^2 - \overline{m})|\overline{m}\rangle = 0 \\
\Rightarrow \quad & \lambda = \overline{m}^2 + \overline{m} \\
\Rightarrow \quad & \underline{m}^2 - \underline{m} = \overline{m}^2 + \overline{m} \\
\Rightarrow \quad & (\underline{m} + \overline{m})(\overline{m} - \underline{m} + 1) = 0 \\
\because \quad & \overline{m} > \underline{m} \\
\therefore \quad & \underline{m} = -\overline{m}
\end{aligned}
$$

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参考内容提纲

内容	参考书
厄米算符	【Lv】§7.2
	【杨】§16 【曾】§4.2
厄米算符的性质	【Lv】§7.3
量子力学基本假设	【Lv】§7.8-7.9
对易子和不确定原理	【Lv】§7.4 【杨】§13 【曾】§4.3
谐振子的代数解法	【曾】§9.1
角动量的一般性质	【Lv】§5.4 【曾】§9.2
表象	【曾】§4.5-4.6
电子自旋	【Lv】§10.1 【杨】§18-20 【曾】§8.1
全同粒子	【Lv】§10.3, 10.5 【杨】§26
He、Li 原子	【Lv】§10.4 【杨】§24
Slater 行列式	【Lv】§10.6
二能级系统	【费恩曼物理学讲义 III】§9.1-9.5